

DAVID GODFREY PETTIFOR CBE

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BY ADRIAN P. SUTTON FRS^{1,*}, RALF DRAUTZ^{2§} AND VACLAV VITEK^{3†}

¹Department of Physics, Imperial College London, Exhibition Road, SW7 2AZ

²ICAMS, Ruh-Universität Bochum, IC 02-521, Universitätsstrasse 150,
44801 Bochum, Germany

³Department of Materials Science and Engineering, 3231 Walnut St.,
Philadelphia PA 19104-6272, USA

* a.sutton@imperial.ac.uk

§ ralf.drautz@rub.de

† vitek@seas.upenn.edu

David Pettifor was a theoretical physicist who changed the nature of materials science by raising the status of materials modelling to that of materials characterisation and processing. He believed that the subject advanced through the development of simple models that withstood rigorous testing against experiments and the most accurate numerical computations. Having been a pioneer of total energy density functional theory calculations, he went on to derive analytic interatomic potentials for transition metals and nearly free electron metals and alloys from quantum mechanical principles. He is probably best known for the development of highly successful structure maps for binary and pseudo-binary alloys that were used by alloy developers in industry to create intermetallic alloys with improved properties. At Oxford he established the first materials modelling laboratory, bringing together physicists, chemists, materials scientists and engineers to model materials across length and time scales, and which became a flagship laboratory for materials scientists world-wide.



Family background

David's father, Percy Hayward Pettifor, and his paternal grandfather, Percy Godfrey Pettifor, were engineers. His father read engineering at King's College London before joining Siemens. When the factory and laboratory were bombed in September 1940 Siemens moved north to Dewsbury where his father was appointed Chief Inspector of their dispersal factory, responsible for all radar and carrier equipment. Towards the end of the war he joined Associated Industrial Consultants (AIC) which took him to Keighley, West Yorkshire, where David was born with his twin brother John in March 1945. The family moved to Purley in Surrey, now South London, in 1947. In 1951 they moved to Johannesburg where his father was asked to build up the AIC operation in Southern Africa.

David's maternal grandfather, Albert Bernard Cotterill, had a reputation for being very good at mathematics. He was awarded a scholarship to attend the Higher Grade School in Hanley, now part of Stoke-on-Trent, where he obtained a first class pass in stage 3 of the South Kensington Board of Education mathematics examination in 1906. He then moved to London and worked for the Inland Revenue. David's mother, Margaret Cotterill, was born in 1917, the eldest of three children. His grandfather died at age 42, so David never met the relative he had the closest resemblance to.

Childhood

David was brought up in a professional, middle-class home in Johannesburg. With his father away a lot on business his mother ran the home. She had high expectations of her four children and they all obtained doctorates: Andrew, the oldest, in Economic Engineering from Stanford, John, David's twin, in Medicine from the University of Witwatersrand, Richard, the youngest, in Ornithology from Oxford, and David in Theoretical Physics from Cambridge. The orientation towards science/engineering was nurtured by their father's subscriptions to *New Scientist* and *Discovery and Endeavour*.

David and John went to St John's College between 1954 and 1962, one of the top three private schools in South Africa. The only places available were in a class one year ahead of their age group. Despite being plunged in at the deep end David excelled and he was awarded prizes across the academic spectrum, with the notable exception of Afrikaans. His favourite subject was English. In 1960 he wrote an essay about the contrasting life in the day of a washer woman from Soweto and a rich housewife from Houghton, which was read out by the Head of English to all three English streams in his year. It may have reflected the underlying unease among whites after Macmillan's 'wind of change' speech to the South

African parliament in February of that year and the subsequent Sharpeville massacre in March.

At school he also enjoyed the chemistry laboratories where he became aware of the importance of the Periodic Table hanging on the wall. Physics was dull. Mathematics came naturally. He decided he wanted to become a physical scientist, making predictions that could later be tested by experiment. He was accepted to read Chemical Engineering at the University of Witwatersrand, but a chance encounter with his physics teacher at the last minute persuaded him to change to reading physics because it was the most fundamental of all the physical sciences, a decision that set the course for his subsequent career.

University



Figure 1: Science students' council 1964, The University of the Witwatersrand. David is in the second row, second from the right. Professor Frank Nabarro is in the centre of the front row. Photo supplied by Di Gold.

David started his undergraduate course as a physics major in February 1963 at the University of Witwatersrand (Wits). In 1953 Frank Nabarro (FRS 1971) left the University of Birmingham to become Head of Physics at Wits. Nabarro rapidly built up the undergraduate

four-year Honours course to an international standard, and set the tone for what was expected of a good scientist. David soon became involved in several student societies and councils, see Figure 1. Although he later abandoned religious belief he was a member of the Anglican Students Federation where he worked with Steve Biko. In September 1965 he was elected by the science students onto the University's Student Representative Council (SRC), where he served for a year on the Executive as the Assistant Treasurer in charge of publications. That year coincided with increased political ferment on campus. The banning of Ian Robertson in May 1966, who was the President of the National Union of South Africa Students, led to massive demonstrations with a march through the centre of Johannesburg and a week-long vigil outside the university gates. In the middle of this unrest Senator Robert Kennedy arrived at Wits as guest of the SRC and gave the speech at the annual Day of Affirmation of Academic Freedom to a packed audience in the University's Great Hall. Sitting on the podium David looked out over a sea of white faces. How very different forty years later when David gave a plenary talk at the South African Institute of Physics annual conference to a packed hall representing a truly rainbow nation.

There was virtually no modern physics in the three-year BSc degree in Physics and Mathematics. It was crammed into the fourth year when the class had shrunk to less than 20% of the original BSc cohort of about 35 physics majors. Having gained a first class honours degree he was offered a research assistantship at the University of California for a masters degree in astrophysics. At the same time he was awarded a South African National Postgraduate Scholarship to study in the UK. At Frank Nabarro's suggestion, Volker Heine (FRS 1974) in the Cavendish offered David a PhD place to do research in Solid State Theory. After all the lectures of his fourth year at Wits he wanted to get stuck into research so he accepted the Cambridge offer and became a solid state theorist rather than an astrophysicist.

Postgraduate research

In his letter of 7th June 1967 to David, Heine wrote about the exceptionally strong group David was about to join in Cambridge:

I would like to tell you a bit about our group. Professor Nabarro has already told you that we shall have a new Professor of Solid State Theory with us next year. His name is Phil Anderson (Nobel Laureate 1977, ForMemRS 1980), and he is one of the two brightest people in the world to appear in Solid State Theory since the second world war. Although he will only be here six months out of every year, there will be someone closely associated with him remaining here all the year round, and who will supervise his research while he is away. There is also Dr. Brian Josephson, (FRS 1970, Nobel Laureate 1973), who is an extremely

bright young theorist. Anderson works on superconductivity and magnetism and Josephson on superconductivity and second order phase transitions in general. I think we should leave it open at this stage as to whom you would be working with exactly i.e. with me or Anderson or Josephson. At the end of September we shall know exactly who is coming and can talk about it all then.

When David arrived in Cambridge at the end of September the interesting projects had already been taken by students who had arrived earlier in the summer. Heine suggested David looked at ‘the long wavelength behaviour of the Augmented Plane Wave pseudopotential’. David was not enthralled. A few weeks later Ross Deegan, who was a visiting Canadian NRC postdoctoral fellow, suggested to David, with Heine’s approval, that he work on understanding the well known structural trend from hcp to bcc to hcp to fcc across the non-magnetic 4d and 5d transition metal series. David was thrilled, not least because for him it was a return to the Periodic Table of his school chemistry laboratory.

Shortly afterwards Denis Weaire (FRS 1999), with whom David shared an office, alerted David to a paper by John Hubbard that had just been published (Hubbard 1967). It was a revelation for David, a beautifully written paper that set the standard David attempted to emulate in all his own publications. Hodges et al. 1966 and Mueller 1967 had demonstrated that the first principles Augmented Plane Wave or Korringa-Kohn-Rostoker (KKR) band-structures of fcc copper and nickel could be reproduced by a physically motivated model Hamiltonian of the hybrid nearly-free-electron tight-binding form (H-NFE-TB). Hubbard 1967 showed that this H-NFE-TB form could be derived directly from the KKR secular equation by performing an Ewald split on the KKR structure constants and by assuming the d electrons scatter resonantly. A year later David published a paper (1) that removed certain inconsistencies in the Hubbard approach that had led to the necessity to retain third nearest-neighbour reciprocal and real space lattice vectors to achieve the desired accuracy for fcc copper. Subsequently David showed (2,3) that second order terms in the model Hamiltonian corresponded directly to the three-centre integrals and non-orthogonality contributions which had previously been neglected. His linearized H-NFE-TB band-structure theory, based on resonant orbitals, was the forerunner for the widely used linearized muffin tin orbital (LMTO) theory developed by O K Andersen. These developments led to powerful computational schemes during the 70s and 80s for the rapid calculation of the band-structures of metals and alloys.

The development of this accurate H-NFE-TB scheme provided the means for David to achieve the goal of his PhD and explain the structural trends across the non-magnetic

transition metals (3,5). Assuming that all three phases had the same atomic volume, they could then be characterised by just two resonant parameters from which the two-centre TB hopping integrals and hybridization matrix elements for the three crystal structures could be calculated directly using his explicit expressions in (1). Away from the noble metal end the predicted structural trend agreed with experiment and was directly related to the filling of the d-band. In January 1970 he met François Ducastelle who showed David the power of analysing structural trends in terms of moments of the density of states, which was also to have a strong influence on David's bond order potentials, sixteen years later.

Postdoctoral research

In October 1970 David started a two-year postdoctoral position with Bryan Coles (FRS 1991) in the Department of Physics at Imperial College. However, after his experiences in South Africa he was undecided whether to pursue a scientific career or to be involved in something more overtly social and political. Edward Heath, the leader of the Conservative Party, had won the 1970 general election and Britain was rapidly becoming a grey place, 'the sick man of Europe'. He did not want to return to South Africa with its destructive atmosphere. Instead he wrote to the University of Dar es Salaam in Tanzania. The country's president, Julius Nyerere, had introduced African socialism several years earlier. They offered David a two-year contract lecturing in the Physics Department starting in January 1972.

He travelled to Tanzania with his first wife Ann. They had met at Wits where she majored in English and they had married on 16 July 1969 in Johannesburg. On arrival in Tanzania he soon became fully involved not only in the physics department but also as a tutor in the University's Development Studies programme where nearly 90% of the physics students were bonded to become teachers, and they spent part of their vacations on teaching practice. In August 1973 he sent a letter to *Physics Bulletin*, published by the Institute of Physics, in response to John Ziman's (FRS 1968) guest leader in the May issue. In the leader Ziman warned against the 'vague aspirations and grand designs' of the World Plan of Action for the Application of Science and Technology to development. In his letter David noted that the Third World had already realised from bitter experience that the technology offered to them by the West was usually divorced from their real needs and costly in its implementation. He warned that the same mistakes must not be made in the proposed transfer of scientific know-how. He argued it was essential for physicists from Third World countries studying in the West to undertake research directly relevant to their countries of origin: '*As physicists we must be honest with ourselves and face the fact that most of our basic research is not needed by developing countries at the present moment.*' The priority of physicists in

under-developed countries, he maintained, should be to build a viable scientific base by concentrating on education from primary school through to university: they *'should realise that physics is not the story of great men working in isolation from the pressures of society, but that science has evolved as the response of man to his external environment'*. He called for an increased awareness of the problems faced by underdeveloped countries so that physicists *'may avoid killing with kindness'*.

During his time in Tanzania he came to the realisation that he wanted to pursue a scientific career. Seeing no long-term future as an expatriate in Tanzania he returned with Ann to the UK. In October 1973 he took up a one-year temporary lectureship in the Department of Mathematics at Imperial College. The following January he met Allan Macintosh who told him about Ole Andersen's ideas of the atomic sphere approximation (ASA) and canonical bands. This meeting led to David spending 3 months with Andersen's group at the Technical University of Denmark Lyngby in the summer of 1974. It was a seminal visit because it gave David a complementary approach to viewing the band-structure problem: rather than starting from phase shifts and scattering theory the ASA started from logarithmic derivatives and the boundary conditions imposed at the atomic sphere boundary. Using this approach he could generalise the classic ideas of Wigner and Seitz for treating the cohesion of alkali metals to that of the transition metals. At that time Andersen was not interested in total energy calculations and he gave David the green light to use the ASA for studying cohesion and bonding on his return to the UK.

David then spent the next three and a half years back in the Cavendish Laboratory as a research assistant. The first year was funded by SRC, the subsequent years by an extramural research contract from UKAEA-Harwell with the metal physics group of Ron Bullough (FRS 1985). The goal was to understand the bonding in transition metals by carrying out some of the very first total energy density functional theory (DFT) calculations, to guide the development of improved interatomic potentials for modelling extended defects in metals such as dislocations (24). Interatomic potentials attempt to fold the dependence of the forces acting between atoms on the local electronic structure into a function, or set of functions, that depends only on the positions of the atoms. As it turned out he succeeded in creating such potentials only later in his life with the development of bond order potentials.

He soon encountered a problem: how to interpret the binding energy which was the difference between two very large numbers, namely the band energy and the double counting term. As Art Williams at IBM Yorktown Heights eloquently put it, it was like finding the weight of a sea-captain by weighing his ship when he is aboard and ashore. The double

counting term in the total energy comprises the Coulomb energy and the exchange-correlation energy, and it cannot be decomposed uniquely into contributions from different orbital angular momenta. But in two seminal papers (6,7) David showed that by working with the pressure, rather than the energy, it was possible to provide a unique separation of the individual s, p and d contributions to the equation of state. This insight had a major impact on the electronic structure community at the time because it enabled the behaviour of the binding energy curves as a function of volume to be linked directly to the known properties of the band-structure.

During his last year in Cambridge David attended a workshop in Liège where Andreas Miedema presented a simple empirical scheme for evaluating the heats of formation of alloys by assembling them from the Wigner-Seitz cells of the constituent metals (Miedema et al. 1973). The scheme successfully separated those alloys with positive heats from those with negative heats of formation by adding a repulsive contribution, that depended on the charge-density mismatch, to Pauling's attractive *ionic* contribution that depended on the electronegativity difference between the constituent atoms. At the same workshop François Gautier presented tight-binding *band* calculations and he obtained heats of formation in reasonable agreement with experiment. David was intrigued by the apparent conflict between these two approaches, one ionic the other band-like. He felt the ASA, which started from cutting out atomic spheres, could provide a sensible approach to resolve the two approaches. He mentioned this thought to Chandra Varma who was visiting the Cavendish at the time. Varma invited David to Bell Labs for six months in the summer to investigate the problem. Within a month or so of arriving in the 'hot-house' that was the theory group at Bell Labs, it became apparent that it was not possible to justify Miedema's empirical scheme from DFT within the ASA. An even more accurate DFT method was needed and none was then available. After months of careful thought he wrote down a simple, back-of-an-envelope, model which captured all the essential physics of the problem. The maths involved was no more than A-level. His model (8) was a generalisation of Friedel's rectangular d-band model for the cohesive energies of pure nonmagnetic transition metals. David's model predicted the heat of formation varied as the square of the difference of the group number of the constituent atoms, but with a pre-factor whose sign depended on the average group number. The predictions of his model agreed with known experimental results, and the physical assumptions of his model were subsequently confirmed by accurate DFT calculations from the group of Art Williams (Williams et al. 1980). This work highlighted David's extraordinary ability to think his way through to the solution of a physical problem, without

getting side-tracked into the development of new computational methods. It illustrated his view (28) that:

‘solving numerically quantum mechanical or classical equations is not the key step in providing insight into the complex world of materials and their properties. The critical step, the creative step, is finding a model that encompasses the dominant mechanisms of the complex process one is wishing to describe.’

Perhaps we can see here the influence of Sir Nevill Mott (FRS 1936, Nobel Prize 1977), who was the charismatic Head of the Cavendish when David was a postgraduate student, and whose portrait hung in David’s office.

Department of Mathematics, Imperial College

David was appointed to a lectureship in the Mathematical Physics group of the Maths Department at Imperial College in October 1978. The Mathematical Physics group was one of the strongest solid state theory groups in the UK at that time. It was led by Peter Wohlfarth and included David Edwards, Alex Hewson, Dennis Newnes, Roy Jacobs and Peter Young. Their research concentrated on magnetism. David had already been made aware of the challenges of magnetism by Peter Miodownik, a metallurgist at the University of Surrey, who had told David about the unique properties of pure iron with its four phases and three crystal structures. This meeting stimulated David’s research on the temperature-pressure phase diagram of iron, which David succeeded in reproducing theoretically in 1983 with Hideo Hasegawa an academic visitor (9).

In the summer of 1980 David was invited by Art Williams and Dan Gelatt to IBM Yorktown Heights as a visiting scientist for a month. Having successfully investigated the heats of formation of alloys of transition metals using DFT they were interested in binary alloys of sp-valent metals such as NaK, NaMg, NaAl, NaSi and MgAl, MgSi and MgP. They asked David whether a simple model could be developed to explain the trends they had calculated in the heats of formation with DFT. He started from second order perturbation theory in real space where the binding energy of a nearly-free-electron metal is the sum of three terms: an electron gas term dependent only on the average density of the valence electrons, an electrostatic interaction of an ion with its own screening cloud of electrons, and the usual pair-potential contribution describing the interaction between an ion and neighbouring screened ions. He found the first term predicted a heat of formation that was proportional to the density mismatch squared but with a prefactor that changed from positive

to negative as the average density of the alloy increased. This accounted for the trend found by DFT calculations, from positive values for the alkali metal alloys NaK and NaRb to the negative values for MgSi and MgP (21). Although the density mismatch term was reminiscent of Miedema's scheme for the heats of formation, David's theory was based on the superposition of *neutral* pseudoatoms in contrast to the *ionic* picture of Miedema's scheme.

This research led him to develop analytic pair potentials for sp-valent metals by replacing the Lindhard dielectric function by a Padé approximant. He showed that the pair potential contribution could be expressed analytically as the sum of three damped oscillatory terms (short-, medium- and long-ranged) in addition to the usual very long-range asymptotic Friedel oscillations (10). This theory provided the first clear distinction to be made between alloys whose structure is governed by Fermi surface nesting with the Brillouin zone in *reciprocal* space, versus alloys whose structure is governed by the oscillatory behaviour of the interatomic potential with respect to the first few neighbour shells in *real* space (29). The former class of alloys includes the Hume-Rothery electron phases with structures controlled by the asymptotic Friedel oscillations, dependent only on the electron per atom ratio. The latter class includes the common nearly-free-electron metals Na, Mg and Al whose structures are dependent not only on the electron per atom ratio but also the phase of the near-neighbour oscillations, and hence implicitly on the ion-core size and valence electron density.

David became interested in structure maps in 1981. He was intrigued by the challenge of finding suitable coordinates for the maps that resulted in a clear separation of the vast experimental data-base of crystal structures into distinct regions, so that all the binary compounds of a particular stoichiometry A_xB_{1-x} with one crystal structure are separated on the map from all those with another crystal structure. This was not just an academic exercise. Developers of alloys for jet engines were searching, essentially by trial and error, for new alloys that could operate at higher temperatures and remain ductile at all temperatures. While alloys with high melting points were relatively easy to find, they usually had crystal structures that made them brittle. A structure map could be used to guide the selection of ternary additions to a pseudo-binary alloy to change its crystal structure into one that is more ductile.

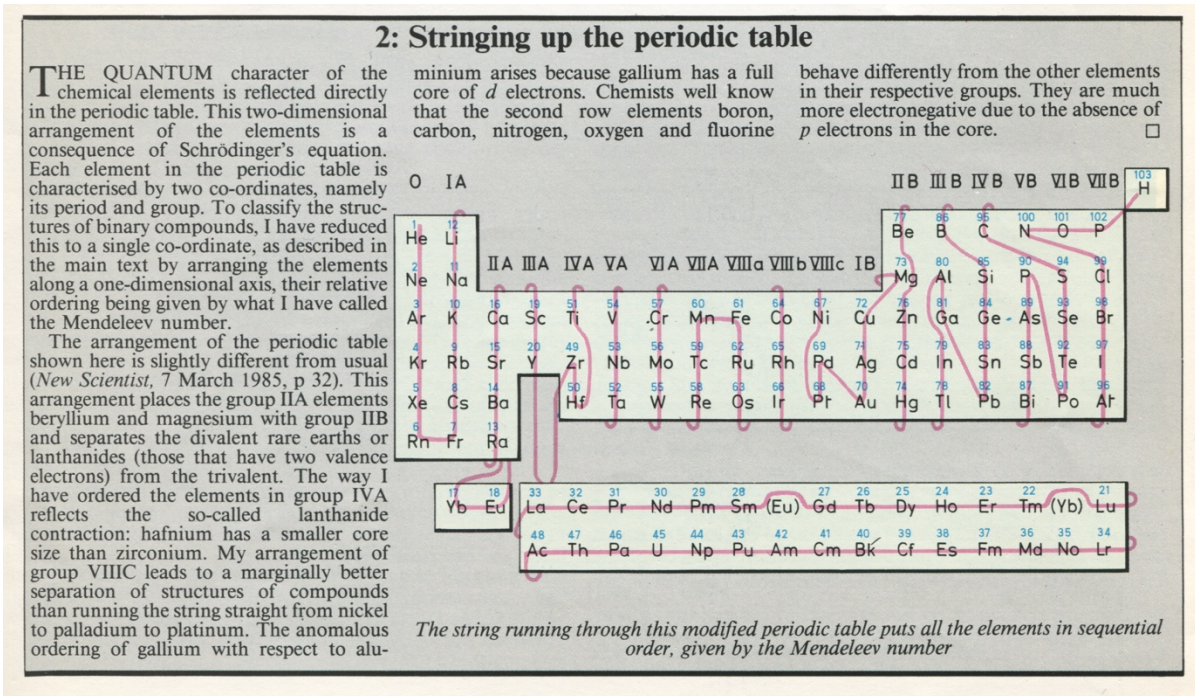


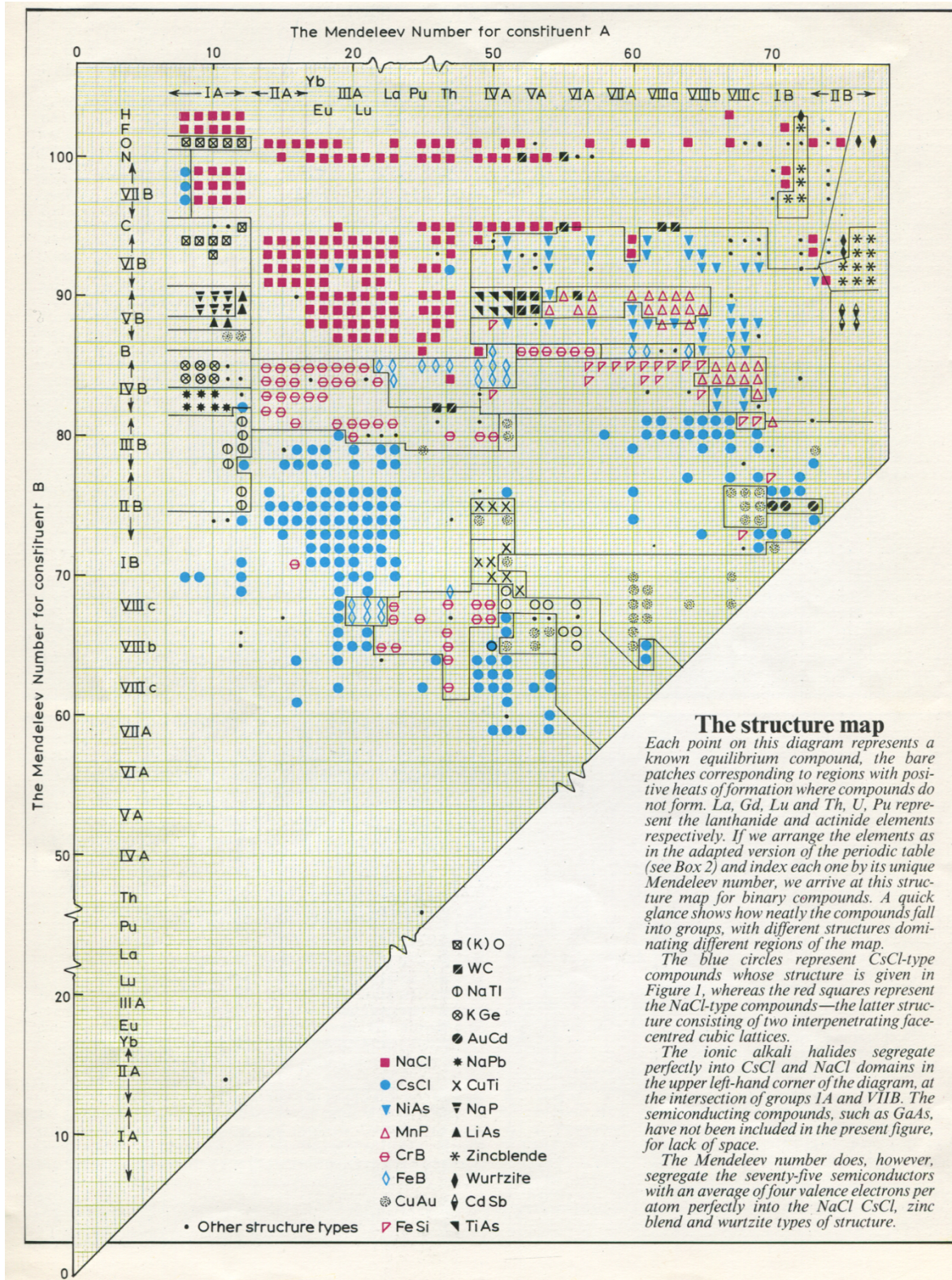
Figure 2: The imaginary string David ran through the Periodic Table for his structure maps. Reproduced from *New Scientist* (13) with permission.

When he started looking at the problem he noticed that the approaches that had been taken were based on finding coordinates that reflected the physical factors thought to underpin structural stability such as the electronegativity difference, the atomic size difference and the average number of electrons per atom. But even with three coordinates the separation of the crystal structures achieved by these maps was not very successful, and with the stoichiometry forming a fourth coordinate the maps were four-dimensional which certainly did not make them user-friendly.

David observed that these three physical factors were essentially classical in origin, and they did not reflect the quantum mechanical nature of the chemical bond. Valence *s*, *p* and *d* orbitals have very different angular characters, which strongly influences the arrangement of neighbouring atoms. To achieve a two-dimensional map for binary compounds with a particular stoichiometry each element had to be represented by a single coordinate. David achieved this by going back to the Periodic Table which had made such a deep impression on him during his school-days in Johannesburg. He assigned to each element just one number, increasing with its position on an imaginary string (see Figure 2), which he threaded through all the elements in the Periodic Table. But this was not the conventional ordering by atomic number or group. Originally he called the number the Mendeleev number, but he later withdrew that label because Frack Nabarro wrote in a letter to David,

dated January 17 1992, that Mendeleev discovered the atomic number and to assign any other number to Mendeleev was 'spurious'¹. He then entered all the elements in this order along the top edge of a large sheet of paper, and again from the top down along the left-hand edge. This was to be his structure map. With a pencil he marked each compound of two elements with a particular stoichiometry as a point on the map. By optimising the ordering of the elements on his imaginary string in a phenomenological way he was able to make compounds sharing the same structure fall into regions which were remarkably well separated from those sharing another structure. Incorporating the Periodic Table into the ordering of the elements enabled him to capture the quantum nature of the chemical bond. The simplicity of these maps was pure genius. In 1986 he was invited to write about them (13) in *New Scientist*. He was thrilled by the invitation and delighted with how the magazine presented his AB structure map in a full-page colour rendition, which is reproduced in Fig.3.

¹ Nabarro was quite wrong. Mendeleev ordered the elements by atomic mass, and it was Moseley who discovered the atomic number in 1913, six years after Mendeleev's death.



The structure map

Each point on this diagram represents a known equilibrium compound, the bare patches corresponding to regions with positive heats of formation where compounds do not form. La, Gd, Lu and Th, U, Pu represent the lanthanide and actinide elements respectively. If we arrange the elements as in the adapted version of the periodic table (see Box 2) and index each one by its unique Mendeleev number, we arrive at this structure map for binary compounds. A quick glance shows how neatly the compounds fall into groups, with different structures dominating different regions of the map.

The blue circles represent CsCl-type compounds whose structure is given in Figure 1, whereas the red squares represent the NaCl-type compounds—the latter structure consisting of two interpenetrating face-centred cubic lattices.

The ionic alkali halides segregate perfectly into CsCl and NaCl domains in the upper left-hand corner of the diagram, at the intersection of groups IA and VIIB. The semiconducting compounds, such as GaAs, have not been included in the present figure, for lack of space.

The Mendeleev number does, however, segregate the seventy-five semiconductors with an average of four valence electrons per atom perfectly into the NaCl CsCl, zinc blend and wurtzite types of structure.

Figure 3: The structure map for binary compounds with stoichiometry AB. Reproduced from *New Scientist* (13) with permission.

UNIVERSITY of PENNSYLVANIA

David P. Pope
Associate Dean
Undergraduate Education
School of Engineering and Applied Science
109 Towne Building
Philadelphia, PA 19104-6391
215-898-7246

February 1, 1988

Dr. Robert Cahn
6 Storey's Way
Cambridge, CB3 0DJ
UNITED KINGDOM

Dear Robert;

I'm writing to tell you about the role that David Pettifor played in last summer's Gordon Conference on Physical Metallurgy that Harry Lipsitt and I chaired. Harry and I tried very hard to bridge the gap between those engineers and scientists who study fundamental properties and those who actually develop new alloys (the theme of the conference was "Ordered Alloys"). To this end we invited a number of theorists who routinely talk to alloy developers: Vvedensky, Freeman, Shore and Pettifor. At the risk of appearing immodest, we were wildly successful, and the high point of the conference was Dave Pettifor's talk. I actually had to enlist my graduate students' to help in coordinating the requests for Dave's reprints! Furthermore, I discovered that Dr. R. Darolia of GE's Evendale (turbine engine) division had begun using a Pettifor map some six months earlier to help him convert a D0₂₂ structure to L1₂ via alloying additions. This was prior to the publication of the maps--he learned of the maps at a prior conference. By the time of the conference Darolia had produced single crystalline alloys of the desired crystal structure and was measuring their mechanical properties.

I believe that the Pettifor maps will prove to be the biggest single recent advance in the field of ordered alloys. In many laboratories around the world researchers are attempting to produce a new generation of tough, strong alloys for use at temperatures above 1100° C. These efforts necessarily involve the manipulation of crystal structure, and the Pettifor maps provide the best rational basis for doing this. Consequently, in less than a year's time the Pettifor maps have become routine tools for workers in the field.

Sincerely,

David P. Pope
David P. Pope

David, I've sent a copy of this to Eric Ash.

R.

Figure 4: Letter from David Pope, University of Pennsylvania, to Robert Cahn, with a footnote from Cahn telling David he had sent a copy to Eric Ash, Rector of Imperial College. Letter supplied by Di Gold, and reproduced here with permission of David Pope.

Pettifor structure maps had an immediate impact on alloy developers, and it is the work for which he is probably best known in the materials science community. This is best illustrated by an unsolicited letter from David Pope to Robert Cahn (FRS 1991), which is reproduced in Fig.4. Cahn copied this letter to Eric Ash (FRS 1977), Rector of Imperial College, and shortly after David was promoted to a professorship of theoretical solid state physics. In 1995 David received the William Hume-Rothery Award by the TMS for proposing ‘*a method of displaying all the data on the ground state structures of binary compounds within a single three-dimensional map*’.

Despite the evident success of the structure maps they did not explain the origin of the different structural domains. For that one needs a theory which takes into account explicitly the quantum nature of bonding in the different crystal structures. For this David used (11) the tight-binding approximation and in 1984 showed, with Raimund Podloucky (a one-year SRC research assistant), that the topology of the pd-bonded AB structure map could be explained by a simple canonical pd-bond TB model using David’s structural energy difference theorem (14) to prepare the atomic volumes. The different roles played by the electronegativity difference, more precisely the valence p and d atomic energy level separation, the relative size difference, and the electron per atom ratio were studied directly (15).

The use of tight-binding invariably attracts derision from DFT purists. Phillips et al. (1985) wrote in a Comment to (11):

The relative merits of microscopic and phenomenological global surveys are to some extent a matter of taste. Because of the small energy differences between crystal structures one might believe that a tight-binding framework such as that used by Pettifor and Podloucky, which cannot predict equilibrium volumes accurately, would not adequately predict structural energy differences. One instead would expect self-consistent calculations using a converged basis set would be necessary.

Pettifor and Podloucky responded (12):

Phillips et al. believe that eventually we must choose between phenomenological and microscopic treatments of structural stability. However, the two approaches perform very different but complementary roles. The phenomenological approach seeks to order the experimental data with the aid of two- (three-) dimensional structure maps. The microscopic approach seeks to explain the origin of the different structural domains within a fundamental

quantum mechanical framework. By attributing the latter role to their phenomenological models, Phillips et al. fall between two stools – neither do they provide the best two-dimensional structural separation of the experimental data nor do they provide the correct microscopic explanation of structural stability.

During the 1980s David made increasing use of the tight-binding approximation, and in his hands it provided unique physical insight and opened new doors. In particular it gave him a path to the development of interatomic potentials for transition metals grounded in quantum mechanics, fulfilling an ambition dating from his postdoctoral days at Cambridge when he was funded by the United Kingdom Atomic Energy Authority (UKAEA) at Harwell. The development of these potentials occupied him for the rest of his life.

The work started in 1986 when he was awarded \$100,000 p.a. for 4 years by the US Department of Energy (DoE), with strong support from the alloy developer C T Liu at Oak Ridge National Laboratory. During the development of the tight binding bond model (16) David had realised there were significant conceptual and mathematical advantages to thinking about how a bond depended on its local atomic environment, rather than an atom. The key quantity to characterise a bond is the bond order, a concept introduced by Charles Coulson (FRS 1950) (Coulson 1939). It is defined as one half of the number of electrons occupying bonding states minus one half of the number of electrons occupying anti-bonding states in a bond. The challenge was to develop a function, which is the bond order potential (BOP), that captured the quantum mechanical dependence of the bond order on the local atomic environment. He showed in 1989 (17) how the bond order in an s-valent tight-binding model could be expressed as a function involving three- and four-body interactions. For David the development of BOPs was his contribution to bridging length scales in modelling materials, in this case between the electronic and atomistic scales.

It was at about the time he started to develop BOPs that his first marriage broke down and was eventually dissolved on 4 September 1990. In 1991 David and his two boys, Thomas (b. 1 December 1973) and Christopher (b. 18 February 1975), from his first marriage set up home with Di Gold and her two boys, Matthew (b. 8 March 1975) and Benjamin (b. 15 May 1977). Di is a successful stained glass artist. David and Di married on 22 May 2004 in Witney, Oxfordshire.

Department of Materials, University of Oxford

In 1992 David moved to Oxford to take up the Isaac Wolfson Professorship of Metallurgy, which he was offered without being interviewed. At the same time he was appointed to a

Professorial Fellowship at St. Edmund Hall. David and Di moved with their four boys to their rural idyll in Charlbury in 1993. While Di worked on her stained glass in their converted barn, David beavered away in his study overlooking Cornbury Park. There was a constant stream of visitors and walks in the glorious countryside around Charlbury. He described Charlbury as paradise, and he was never happier than when he was with family and friends at home sharing a bottle of wine and a hearty meal with lively conversation.

David had a clear idea of what he wanted to achieve at Oxford. His goal was to establish a materials modelling laboratory (MML) to model materials theoretically and computationally across length and time scales in collaboration with the strong experimental groups within the department and with industry. Although he was a theoretical physicist he understood very well that the science and engineering of materials is a multidisciplinary activity involving physicists, chemists, materials scientists, computer scientists and engineers. Today one would add biologists and mathematicians. To realise his vision he had to break down the silo mentality where physicists and chemists work at the electronic and atomic scales, materials scientists work at the microstructural scale, and engineers work at the macroscale of components. He also recognised that the greatest intellectual challenges lay in the transfer of information between the silos, for which his bond order potentials were an outstanding example.

Not surprisingly he met considerable resistance from his new colleagues when he asked them to get involved. They did not understand why he wanted to call it a Materials *Modelling* Laboratory and not a Laboratory for *Computational* Materials Science. They teased him about using plasticine for his modelling. But for David it was only through the development of models '*as simple as possible but not simpler*' that one can hope to reach an understanding. The quotation is widely attributed to Einstein, and it appears above the preface in his book (21). Heavy number crunching was essential, but only to check one's understanding embodied in simple models. Having pioneered some of the first total energy DFT calculations in the seventies he was well qualified to hold this view. It led him often to remark that it was not more computing power that the subject needed but more good models.



Figure 5: Launch of the Convex supercomputer in the Materials Modelling Laboratory on May 23 1997. Left to right: Professor Brian Cantor Head of Department of Materials, David, Dr Bill Hayes Pro-Vice Chancellor, Dr Joel Birnbaum Senior Vice President for Research and Development at Hewlett-Packard (HP), Mr Pierre-François Catté General Manager of HP Convex Division. Reproduced from *The University Gazette*, University of Oxford, with permission. Seven months later David was diagnosed with multiple myeloma.

David set up Friday lunch-time MML seminars to get people talking about modelling and experimental work at different length and time scales, and in a few years they became more popular than the regular departmental colloquia. He developed a very successful collaboration with Hewlett-Packard Labs in Palo Alto which funded three postdoctoral research assistantships for ten years. They worked on a wide range of challenging materials problems of interest to the company, for which he involved several members of staff as supervisors of the research. Eventually he managed to persuade fifteen primarily experimental colleagues with an interest in modelling to be co-investigators on a successful proposal to secure an HP-Convex Exemplar Supercomputer for the MML. The research covered seven areas: materials processing, plasticity, tribology and adhesion, surface structures and reactions, lightweight alloys, biomaterials, and magnetic materials for information storage and sensors. The £726,000 proposal was 50% funded by the Higher Education Funding Council Office for Science and Technology (HEFC/OST) Joint Research Equipment Initiative and 50% by Hewlett Packard's Convex Division, Information Storage

Group, and Corporate Laboratories. On 23rd May 1997 the supercomputer was inaugurated by Dr Joel Birnbaum, the Senior Vice-President for Research and Development at Hewlett-Packard Company, see Fig.5. David had realised his vision. Modelling materials rapidly became recognised world-wide as a vital component of the science and engineering of materials, equal in status to characterisation and processing of materials. In 1999 he received the Royal Society Armourers and Brasiers Company Award for his structure maps and for his ‘*vision and leadership in establishing the Materials Modelling Laboratory at Oxford with its strong links to industry and recognized as an international flagship laboratory for modelling.*’ In 2005 he was awarded a CBE for services to science.

By 2005 David’s work on BOPs had advanced very significantly. In the early nineties he had shown that BOPs for intermetallic alloys and sp-valent materials (18,19) could capture the crucial *angular* dependence of atomic interactions in these materials. Together with Masato Aoki he showed that the perturbation expansion of the original BOP publication (17) could be cast into an exact form (20), which was implemented by Andrew Horsfield in the OXON (Oxford Order N) code (22).

Until the development of BOPs, bond orders were determined by diagonalizing the tight binding Hamiltonian matrix, a computational task that scales as the cube of the number of atoms in a periodically repeated cell. In contrast the bond orders in a BOP are determined in a manner that scales linearly with the number of atoms in the model (BOPs are an ‘O(N) method’), and periodic boundary conditions are avoided. This is achieved by using the recursion method (Heine 1980) to write local electronic Green’s function matrix elements *between* atoms as continued fractions with coefficients expressed in terms of moments of the local tight-binding Hamiltonian in real space. In addition, unlike methods based on finite clusters of atoms the Green’s function matrix elements are embedded in an infinite system, thereby avoiding spurious effects due to free surfaces of a finite cluster. The linear scaling with the number of atoms and the embedding in an infinite system are essential for calculations of the structure and dynamics of extended defects in real space without the crippling limitations of periodic boundary conditions applied to enormous supercells. The first generation of BOPs required the numerical integration of response functions and consequently they were called numerical BOPs. They were used extensively to model dislocations in transition metals and intermetallics (23, 25), particularly by Vaclav Vitek’s group at the University of Pennsylvania. Their development led to the award of a highly prestigious international grant by the New Energy and Industrial Technology Development Organization (NEDO) in Japan to the group comprising David leading the theory, Vaclav

Vitek leading the computer modelling, and David Pope (University of Pennsylvania) and Masaharu Yamaguchi (Kyoto University) leading the experiments.

In 1998 David derived a fully analytic expression for the bond-order potentials from a bond-based, two-level recursion algorithm for the σ and π bonds in sp-valent systems (26). These ‘analytic BOPs’ were applied in collaborations with Jim Butler and Haydn Wadley for modelling hydrocarbons and GaAs respectively, with funding from the Defence Advanced Research Project Agency (DARPA) and Office of Naval Research (ONR).

In a collaboration with Ralf Drautz, David obtained analytic BOPs for transition metals in 2005 by expanding the density of states into Chebyshev polynomials, which avoided numerical integration (30). The analytic framework enabled exact forces to be calculated so that large scale molecular dynamics simulations became possible. An extension to include non-collinear magnetism followed (31). The analytic BOPs were implemented in the BOPfox program which enables massively parallel simulations with millions of atoms (32).

David made significant efforts to bring his ideas to a wider audience. In 1995 his book *Bonding and structure of molecules and solids* (19) appeared. It is aimed at final year undergraduates and first year postgraduates in physics, chemistry and materials science. It is a beautiful introduction to many of his ideas, written with his characteristic clarity and physical insight. In 1997 he published an article for school teachers in *Physics Education* (24) about bridging the gaps between physics, chemistry and engineering in materials modelling. He wrote similar articles in *New Materials* and *Scientific Computing World*. He also published a user-friendly review on *Electron theory in materials modelling* in the Golden Jubilee issue of *Acta Materialia* (29).

In December 1997 disaster struck. He became seriously ill with multiple myeloma at the age of just 52. His height was reduced by four and a half inches as his spine collapsed causing enormous pain. He considered taking early retirement, but in June 2001 the department offered him the possibility of dropping most of his administrative duties, to allow him to focus on his research. His research thrived, and his graduate students and research assistants frequently made the journey to Charlbury. He always expressed his deep gratitude to the department for giving him this opportunity. On 28th April 2003 he gave a talk in Oxford to the Haematology Nurses Forum about his experience of myeloma. The nurses showed their appreciation in the feedback: “Fantastic. Insightful. Brave and moving”, “An invaluable perspective – thank you so much”, “Powerful, moving story. Articulate and so

inspiring”, “Amazing chap”. Over the course of the next 20 years he underwent a succession of chemotherapy treatments which inevitably took their toll, but he never complained and he just got on with it.



Figure 6: David and Di in Charlbury on their way to the Royal Society Summer Science Exhibition 2015. Photo supplied by Di Gold.

Following Nelson Mandela’s release from prison the Royal Society established in 1996 a partnership with the National Research Foundation in South Africa to help build up centres of excellence in previous black universities. David was involved with Richard Catlow (FRS 2004) in helping to set up a Materials Modelling Centre at the University of Limpopo (formerly University of the North, formerly Turfloop in the apartheid era). He returned to South Africa every year after 1996 until his ill health prevented him.

After his retirement in 2010, at age 65, he continued to work with his research group and publish a few papers a year until his health declined further in 2016. His last visit to the Royal Society summer science exhibition, which he always enjoyed, was in 2015 – see Fig.6.

He loved the reunions in Charlbury of his ever-growing family – see Fig.7. He is survived by his wife Di, his sons Thomas and Christopher, and his stepsons Matthew and Benjamin.



Figure 7: David being shown the wonders of an ipad by Django his grandson, with his wife Di looking on and Teddy, another grandson, peeping from behind. Photo supplied by Di Gold.

Personality

On July 10-11, 2018 a two-day meeting was held at St Anne's College, Oxford to celebrate David's life and work, with nineteen talks by scientists from France, Germany, Switzerland, South Africa, the UK and the US. Half way through the science meeting a three-hour memorial meeting took place attended by friends and family as well as scientists. The following edited extracts from speeches at the funeral and from the memorial meeting give a flavour of what it was like to know David as a brother, a father, a friend and a colleague.

John Pettifor, David's twin brother, stated that 'It is in Oxford that I believe he was happiest and most content. He was fulfilled in his academic activities, enjoying his research, his regular formal and informal meetings with his postgraduate students, his international conferences and his sabbaticals in the US. But it was not only his academic activities – in Charlbury he found peace and fulfilment in his family life. From the outside, it appeared that David and Di had an idyllic existence, even if their children might have hankered after the

excitement of London. Whenever I arrived to spend a night on my way to or from a conference, the house was full of their children and partners and their grandchildren. Dinners/lunches were always events with lots of noise, much discussion, plates piled high and lots of wine. But one paid for the meal – you were expected to join David on a brisk walk around the fields of Charlbury afterwards; Christmas days and New Year’s days were not exempt.’

Tom Pettifor, David’s older son, recalls that ‘Now I know it was ... in the mid 1980s that he was reaching perhaps the peak of his career. Dad had an ability to concentrate, he would work for hours in deep thought, elbows on his desk, in his study in 39 Caldervale Road, scribbling mysterious squiggles on sheet upon sheet of paper. Chris and I proudly told everyone that Dad had “cracked it” after he completed his ground-breaking structure maps.’

Ian Evans was a close friend from childhood who records that ‘David and John and I did much together. For a long time, the twins could both fit on my bike, John on the rack behind, and David on the handlebars. In that era, Emmarentia Dam was a wild place, and we’d spend the day fishing, hunting for the crabs that stole our mealie meal bait off our hooks, and eating baked beans. But what is perhaps most unique in my memories of the 64 years is that despite the fame and academic accolades and his exceptional intellectual brilliance, he was always the same cheerful, unassuming, wine-loving, altruistic, principled person who insisted on counting out the exact number of tinned peach halves when we divvied up the dessert on our camping trips.

Shortly after his first treatments I arrived for a visit. David was on the platform at Charlbury station to meet me, and I barely recognized him—shorter than ever, bent, most of his hair gone, and clearly in pain. We walked up the hill to Sheep Street, conversing enthusiastically as though nothing were the matter. His indomitable spirit continued throughout his long illness, with the consistent wonderful support of Di.’

Tony Readhead was a fellow student at the University of Witwatersrand and close friend: ‘Of the many things I loved about David, the most important of which were his intellect and integrity, which became obvious within a few minutes of meeting him, I most particularly appreciated David’s ability to focus absolutely on you when you were talking to him, and the deep interest he showed in everybody he interacted with. I have only known two other people who possessed this quality to the degree that David did – my own father and Martin Ryle. I

also loved David's great sense of humour, which was always bubbling just below the surface. I also loved the mischievousness in David's nature, which often came out quite unexpectedly - it didn't matter whether he was dealing with friends, or colleagues in the Royal Society, the chef at a good restaurant, or a checkout clerk at a liquor store in southern California.

By the time of my 21st birthday David was my closest friend, and he gave me the wonderful gift of Bertrand Russell's *The Wisdom of the West*, with an inscription as follows: "Tony – Congratulations and many thanks for being such a wonderful friend", followed by a quotation from George Eliot:

"It is hard to believe that anything in this world is worthwhile, unless there is some eye to kindle in common with our own, some brief word uttered now and then to imply that what is infinitely precious to us is likewise precious to another mind."

Mike Finnis was a friend and colleague of David's: 'Besides his vision, an outstanding quality was his ability to focus on a problem, concentrating his mind on it, stripping away what was not essential to understanding the situation. He extracted from the evidence the essentials that he found interesting or challenging or what he needed to move his deliberations forward. Conversations were also characterised by this focus. When he was explaining something, he would stop after a couple of sentences and fix you with that piercing look until he felt sure you were following him before he carried on or backtracked to help you. It could be hard work. But he focussed when he was listening too. If you were explaining or presenting an idea to him, he would interrupt with a "hold on, what do you mean by..."', and you'd better know what you were talking about, whatever the subject.'

Ralf Drautz was a friend and colleague of David's: 'David would rarely accept no for an answer. Several times it happened to me that I tried to solve a problem for days and weeks and convinced myself that it just could not be solved. David would listen carefully and patiently and then ask me to try again. And often, with David's intervention, I would finally crack the problem. At times this made me feel really small, but I soon realized I was dealing with a giant. One can only fully appreciate the man David was if one takes into account how incredibly hard he fought. How difficult it must have been for him to remain focused on the small details of a manuscript or a scientific discussion. But he always was focused. There was never the slightest sign of self-pity. He just did not give in.'

Final thoughts

In closing we offer three observations. The first is that there are now many more researchers working on the *methods* of computational materials science than those advancing fundamental understanding of materials through the development of successful simple *models*. This is almost certainly because the skills required to develop methods do not include a deep understanding of materials physics. The development of methods has become an end in itself with many scientists making successful careers out of it. There is no question that David appreciated the importance of developing new computational methods for modelling materials. Indeed he contributed a good deal of method development himself, with his pioneering total energy DFT calculations and methods in tight binding that scale linearly with the number of atoms. But in contrast to so much of current method development, he always had questions in mind about the physics of materials that necessitated the development of his methods. It also seems very unlikely that he would be comfortable with the rise of machine learning and data mining in materials science, not least because there is no model to provide a framework on which to build understanding. For David if there was no model there were only numbers.

Secondly, it is striking that David received significant funding from overseas at critical stages in his career. Funding from the United States DoE, DARPA, ONR, HP Laboratories in Palo Alto and NEDO in Japan enabled him to undertake ambitious, high risk research.

Finally, the overlap between the research of William Hume-Rothery (FRS 1937), the first Isaac Wolfson Professor of Metallurgy at Oxford, and David's research is also striking. Even though H-R was an experimental chemist and David was a theoretical physicist they shared a deep interest in the structural stability of metals and alloys throughout their careers. David never met H-R but he had the highest regard for him, and in 2000 he wrote a wonderful biography about him (27).

Honours and awards

- 2010 Emeritus fellowship of St Edmund Hall, University of Oxford
- 2005 Awarded CBE
- 2005 Symposium in honour of his 60th birthday, Oxford
Proceedings published in Progress in Materials Science **52** (2007), 131-464
- 1999 Royal Society Armourers and Brasiers Company Award
- 1995 William Hume-Rothery Award, The Minerals, Metals and Materials Society (TMS)

- 1995 Elected to Academia Europea
- 1994 Elected FRS
- 1990 Hume-Rothery Prize, The Institute of Metals
- 1989 Elegant Work Prize, The Institute of Metals
- 1986 Medal for contributions to alloy theory, National Research Institute of Metals, Tokyo
- 1965 William Cullen Medal for Most Distinguished Graduate

Named lectures

- 1995 Robert Maddin Lecture in Materials Science, University of Pennsylvania
- 1990 Mott Lecture, Condensed Matter and Materials Physics Conference, Institute of Physics
- 1989 Hume-Rothery Memorial Lecture, University of Oxford

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FIGURE CAPTIONS

Figure 1: Science students' council 1964, The University of the Witwatersrand. David is in the second row, second from the right. Professor Frank Nabarro is in the centre of the front row. Photo supplied by Di Gold.

Figure 2: The imaginary string David ran through the Periodic Table for his structure maps. Reproduced from *New Scientist* (13) with permission.

Figure 3: The structure map for binary compounds with stoichiometry AB. Reproduced from *New Scientist* (13) with permission.

Figure 4: Letter from David Pope (University of Pennsylvania) to Robert Cahn, with a footnote from Cahn telling David he had sent a copy to Eric Ash, Rector of Imperial College. Letter supplied by Di Gold.

Figure 5: Launch of the Convex supercomputer in the Materials Modelling Laboratory on May 23 1997. Left to right: Professor Brian Cantor Head of Department of Materials, David, Dr Bill Hayes Pro-Vice Chancellor, Dr Joel Birnbaum Senior Vice President for Research and Development at Hewlett-Packard (HP), Mr Pierre-François Catté General Manager of HP Convex Division. Reproduced from *The University Gazette*, University of Oxford, with permission. Seven months later David was diagnosed with multiple myeloma.

Figure 6: David and Di in Charlbury on their way to the Royal Society Summer Science Exhibition 2015. Photo supplied by Di Gold.

Figure 7: David being shown the wonders of an ipad by Django his grandson, with his wife Di looking on and Teddy, another grandson, peeping from behind. Photo supplied by Di Gold.



Adrian Sutton FRS is Emeritus Professor of Nanotechnology in the Department of Physics at Imperial College London. Educated in materials science at the University of Oxford and the University of Pennsylvania, he started to collaborate with David Pettifor in 1985 on the tight-binding bond model for covalent and metallic materials. He was appointed to a lectureship in the Department of Metallurgy and Science of Materials at Oxford University in 1991, one year before David became the Isaac Wolfson Professor of Metallurgy in the same department. He shared David's vision of setting up the Materials Modelling Laboratory in Oxford and helped David to realise it. In 2005 he moved to the Department of Physics at Imperial College London where he was one of four Fellows of the Royal Society who founded the Thomas Young Centre (www.thomasyoungcentre.org), involving hundreds of researchers in theory and simulation of materials in chemistry, engineering, materials and physics departments across four London colleges. He also founded and directed the EPSRC Centre for Doctoral Training on Theory and Simulation of Materials at Imperial College (www.tsmcdt.org), which has attracted theoretical physicists, engineers and chemists into theory and simulation of materials, with strong links to manufacturing industry. In 2018 he retired from academic life to concentrate on writing and consulting.



Ralf Drautz is director of the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) at the Ruhr-Universität Bochum, Germany. He obtained his PhD from the Max Planck Institute for Metals Research and the University of Stuttgart. Density functional theory calculations were the workhorse for his research during his PhD. It was when he was searching for a numerically efficient but mathematically accurate and elegant model of atomic interactions in materials that he first came into contact with David Pettifor's work on Bond Order Potentials. Ralf joined David's group at the University of Oxford as a postdoctoral research assistant in 2003. Together with David he developed analytic Bond Order Potentials for transition metals, including magnetism and charge transfer. He continued to work on coarse graining from density functional theory to tight binding and Bond Order Potentials when he became the first director of the newly established ICAMS in 2008. The close collaboration with David led to more than 25 joint publications from 2003 to 2018.



Vaclav Vitek is Harold Pender Professor of Engineering and Applied Science in the Department of Materials Science and Engineering at the University of Pennsylvania. He is a member of the US National Academy of Engineering. He started his research at the Czech Academy of Sciences in Prague, followed by seven years as a research associate at Oxford University, one year as a visiting professor at University of Groningen and one year as the Humboldt Senior Fellow at Max-Planck Institute in Stuttgart. He has also been a visiting researcher at a number of other centres around the world. From the mid-sixties he pioneered some of the first atomic level modelling of crystal defects that control the mechanical properties of metallic materials, notably dislocations, grain boundaries and cracks. The early models used simple empirical potentials to describe interactions between atoms. But even at this stage Vitek dreamed of modelling transition metals, including iron, with a quantum mechanical description of bonding. This dream became a reality when he met David Pettifor in 1990 and learned about bond order potentials. Their collaboration followed and Vitek and his students published with David and his collaborators around twenty-five papers on dislocations and grain boundaries in bcc refractory metals, iridium, hcp titanium and intermetallic compounds using bond order potentials. Several of Vitek's former PhD students are now advancing atomistic modelling of defects in metallic materials based on David's bond order potentials.