but the present discovery is by no means all negative: the local electronic structure in the twisted AA domains is actually unique in its own right, with small electron and hole pockets of distinct pseudospin texture. In fact, it will be important to consider the possibility and implications of such structural defects in the on-going discussion about the true electronic ground state of bilayer graphene where interaction-driven deviations from the single-particle electronic structure are of great interest. Thus, studying and exploiting the electronic consequences of the small twist and similar structural defects might well become an interesting research direction in its own right. ❑

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INTERFACE SUPERCONDUCTIVITY

Pinning the critical temperature

The critical temperature of most superconductors varies with the density of charge carriers, which in turn is most easily tuned by chemical doping. The observation that a specially fabricated two-dimensional superconductor maintains the same critical temperature regardless of doping raises some important questions.

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One of the more widely quoted 'known facts' about superconductors is that their critical temperature, T_c, depends on the density of charge carriers, n. Both the cuprate and the iron pnictide superconductors, as well as a number of 'heavy fermion' materials, display a 'superconducting dome' in the phase diagram, an inverted parabola that traces the relationship between T_c and n, which is common to all these systems. Although the precise origin of this behaviour probably varies from one class of materials to another, it has become natural to expect that the T_c of a superconductor can be maximized by finding an optimal doping value.

Writing in Nature Materials, Ivan Božović and colleagues now report a surprising departure from this picture in bilayer samples consisting of strontium-doped lanthanum cuprate[1]. By means of a combinatorial fabrication approach they prepared interface superconductors at the boundary between two non-superconducting cuprate materials, and found that their T_c remains constant over a wide range of strontium doping.

Our knowledge of the doping dependence of superconductors is mainly based on bulk materials. The essential feature of the $La_{2-x}Sr_xCuO_4$–La_2CuO_4 bilayer samples studied in the present work is that they are truly two-dimensional, in the sense that the active superconducting material consists of a single interface boundary between two insulators with a thickness of one unit cell. The authors note that the chemical potential, μ, of the conduction electrons in these materials is very weakly dependent on doping over a wide range of charge-carrier densities. They therefore propose a model in which the carrier density is redistributed in such a way that, although it can vary across the whole heterostructure, it stays pinned at a constant value in the vicinity of the interface CuO_2 layer.

The notion that the chemical potential is independent of the charge-carrier density over a range of dopings also has ramifications of a purely thermodynamic nature. Because the free energy must be a smooth function of n, the latter parameter is bound to μ and to the compressibility, κ, of the electronic liquid by the well-known Maxwell relation $n^2 \partial\mu/\partial n = -1/\kappa$. Therefore, if the chemical potential is independent of charge-carrier densities over a certain range, then this implies that over that same range the compressibility must be infinite. Such singularities are typical of phase-separation phenomena at liquid–vapour phase transitions. From a microscopic point of view, this requires that the pressure, $p(n)$, has a non-monotonic dependence on n, as illustrated in the middle panel of Fig. 1. From standard thermodynamics it then follows that μ of the system studied by Božović and colleagues also has a non-monotonic charge-carrier-density dependence, as shown in the top panel, and that there is a region of negative compressibility (bottom panel). In thermodynamic equilibrium, the system avoids this unstable situation by separating into two phases, one more dilute (A) and the other more dense (B).
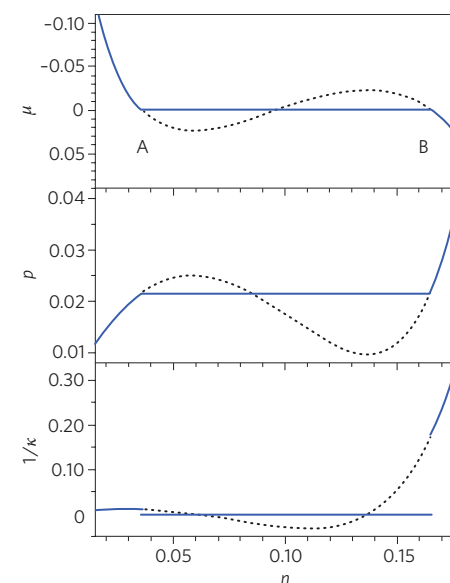

Figure 1 | Illustration of the density dependence of the chemical potential, pressure and inverse compressibility of a fluid undergoing a first-order phase transition (blue solid lines). The black dotted lines are isotherms of the chemical potential ($\mu(n)$; top), pressure ($p(n)$; middle) and inverse compressibility ($1/\kappa(n)$; bottom). The peaks and troughs in the middle of the blue lines indicate a thermodynamical unstable region, where the fluid is replaced by a mixture of two phases, A and B, having the same Gibbs free energy. In the region of coexistence $\mu(n)$, $p(n)$ and $\kappa(n)$ are independent of doping, and the compressibility of the mixed phase is infinite, causing $1/\kappa$ to jump discontinuously at the critical densities n(A) and n(B). All parameters are in arbitrary units.

In ordinary fluids, the liquid–vapour transition arises as a result of the van der Waals interaction between the molecules. In the case of the cuprate superconductors, the possibility of phase separation in various different incarnations has been the subject of intense theoretical and experimental research, most notably concerning striped states of unidirectional modulations of charge and spin ordering[2–10]. Broadly speaking, this is understood as a consequence of the long-ranged Coulomb interaction, which becomes relevant when the electrons become distributed inhomogeneously in puddles of higher and lower density. According to this scenario, the puddles with higher density (corresponding to B in the figure) form a percolating network of electrons having the 'optimal' n corresponding to a T_c of 40 K. Because the present experiments are carried out on a two-dimensional electron fluid, it will be especially important to carefully consider the physics of screening of the Coulomb interaction at an interface, a situation that is geometrically quite distinct from the interior of a bulk crystal.

Further experimental and theoretical research will be required to settle whether the chemical potential is fully doping-independent as these experiments suggest, and indeed whether or not phase separation occurs in these systems. What remains clear is that, in the lively world of superconductivity, new surprises are never too far away. ❑

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MATERIAL WITNESS

AND THE WINNER IS…

How much materials science can be done purely at the computer? More than you could ten years ago, surely, just as it has been for every decade since the computer was invented. But curiously, it's not exponentially more: the extent of what can be predicted by computational methods hasn't scaled with Moore's law. Partly this is the curse of simple volumetrics: an order of magnitude increase in the dimensions of a simulated system corresponds to three orders of magnitude more atoms (and for various reasons the computational intensity can increase still faster). It's also a question of complexity: for example, many materials properties involve dynamic non-equilibrium phenomena that unfold over long timescales.

For these and other reasons, designing materials computationally is still a challenging, often overwhelming task. But it is happening (S. Curtarolo et al. Nature Mater. **12**, 191–201; 2013) — it has become possible, for example, to speak meaningfully of first-principles metallurgy, in which alloys are designed for structural and electronic applications, generally based on density-functional calculations of the relevant bulk properties.

One of the biggest problems for all approaches to materials design, whether experimental or computational, however, is that the range of options is so vast. Even screening ternary alloys presents a dizzying number of candidates, while today's engineering alloys can have ten or more elemental components. The hope here is that computation can at least winnow the list of candidates, even though it's often necessary to resort to experimental testing of the best ones.

But what does 'best' mean? Designing materials has always been a question of compromise, trading one desirable property against another (and cost must almost always be factored in somewhere). It is within this context that Lejaeghere et al. present a new methodology for selecting the best candidates from computational screening of materials (Phys. Rev. Lett. **111,** 075501; 2013). They point out that, although one can often use computation to identify a set of materials that outperforms the rest for a particular set of selection criteria, it is harder to rank these candidates in terms of their optimality. This is what the new procedure accomplishes.

It does so by defining a 'win fraction' for each pair of candidates, which quantifies the fraction of the trade-off in design criteria that favours one candidate over the other, summed over all the criteria. Then the minimum of the win fraction for each candidate with respect to all the others provides the required ranking factor: the larger this minimum, the

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better the trade-off in comparison to the rest of the set.

Lejaeghere et al. show that their approach produces intuitively sensible results when searching among tungsten, its binary alloys, and other pure elements, for economical materials with high mass density. Furthermore, they use the same candidate set to identify materials that optimize hardness (for which the computed bulk modulus stands proxy), thermal resistance (cohesive energy) and price. A third, more demanding case, seeks a material needed in nuclear reactors that balances ductility, temperature resistance and price.

Including more complex materials formulations, or examining properties that demand more than a scale-independent density-functional calculation of bulk properties, will doubtless introduce a steep gradient in computational cost. But at least for certain types of problem, the method can find the best of the bunch. ❑