exceptional agreement. In addition, agreement is good for the theoretical and experimental probabilities for the dissociation reaction that accompanies chemisorption of H_2 on platinum (illustrated in Fig. 1). This is strong evidence for the applicability of the theory. The comparison also suggests that an electronically adiabatic theory – a theory that considers electronically excited states as insignificant — is sufficient to predict and explain the experimental observables for this reaction.

Examination of the potential energy surface provides an explanation as to why the electronically adiabatic theory is sufficient. The energy available to the reactants is not significantly enhanced as the chemisorption energy is relatively small. This seems to be a general feature for the interaction of H_2 with metal surfaces. It is related to the fact that H_2 cannot easily accept electrons from the metal, in contrast to molecules such as NO. Other calculations on the probability of electronic excitations in H_2/metal systems confirm this view[7].

The one slight weakness is that density functional theory has been used to calculate the potential energy surface. Comparison with highly accurate ab initio quantum chemistry calculations for simple gas phase reactions shows that density functional theory does not always predict reaction barriers accurately[8]. But the extensive comparisons that have now been done between theory and experiment for the H_2/metal system do suggest that the density functionals used for this system are reliable.

The conclusions of this study are good news for the theoretical treatment of scattering and reactions of molecules such as H_2 on metal surfaces. The use of the idea of the potential energy surface has held up well and the prospects for extending this type of rigorous quantum theory to other molecule–surface systems are promising. This might include dissociations of more complicated — and highly industrially relevant — molecules such as NH_3 and CH_4 on platinum and other metals.

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MATERIAL WITNESS

Higher T_c?

To the casual observer, high-temperature superconductivity seems to have gone off the boil. In the late 1980s it was the hottest topic in physics, thanks to the discovery in 1986 by Georg Bednorz and Alex Müller of superconducting transition temperatures (T_c) of around 35 K in a class of copper oxides. In 1993 the record reached 133 K.

But that was pretty much as hot as things got, and it seemed as though the task for the coming years was that of meeting the engineering and materials challenges involved in making useable wires from the brittle, polycrystalline ceramics. The excited talk of 'room-temperature superconductors' seemed to fade away.

Such speculation was not new to the high-T_c materials, however. In 1965 Bill Little at Stanford suggested that room-temperature T_cs might be achieved in conjugated organic polymers. Building on the so-called BCS theory that explained superconductivity in terms of electron-pairing mediated by vibrations of the crystal lattice (phonons), Little proposed a new pairing mechanism that involved polarization of polymer side-chains. Because this required the motion of electrons rather than atoms, it might happen at higher temperatures.

Nothing like Little's mechanism has been observed. But it seems clear that, even if the mechanism of superconductivity in high-T_c copper oxides remains poorly understood, it does not involve phonon-mediated interactions. What's more, the limitations of the BCS mechanism seemed themselves to be challenged by the discovery in 2001 of phonon-mediated superconductivity at 40 K in magnesium diboride (MgB_2).

That was one motivation for a workshop last June at the University of Notre Dame in Indiana on the possibility of room-temperature superconductivity. Among the participants was theorist Warren Pickett of the University of California at Davis, who has now released two papers exploring the idea (http://www.arXiv.org/abs/cond-mat/0603482 and cond-mat/0603428). Pickett considers what is needed in a material that shows BCS-like photon-mediated superconductivity with much higher transition temperatures than those currently known.

MgB_2 provides some vital clues. "The truly remarkable aspect of this queen of superconductivity's personality traits is her complete and utter scorn for the conventional wisdom" Pickett says. Unlike previous phonon-mediated materials it has a two-dimensional conduction-electron band and has no *d* electrons. Most importantly, it does not show particularly strong electron–phonon coupling — except for a crucial 3 per cent of the phonons.

In other words, if MgB_2 were able to make fuller use of its phonons, its T_c could be enormous. By considering what this requires of the electronic band structure, Pickett comes up with something like a prescription for very-high-T_c materials. Layered, lithium-doped metal salts of the type Li_xMNCl are promising candidates. Whether or not such a material will ever be found, Pickett says, calls now for neither gloom or glee, but cautious patience.

Philip Ball