is a consequence of Pauli repulsion — the fact that a closed electron shell repels any other electrons. At transition-metal surfaces, the most loosely bound electrons can get out of the way of the incoming H_2 by converting into d -electrons that are strongly localized about the metal atom cores. This is impossible on simple metals (Al, Mg) which have no d -levels, and on noble metals (Cu, Ag, Au) whose d -shells are full. But it is possible on transition metals, because their d -electron shells are 'open', or incomplete.

This argument qualitatively explains the catalytic inactivity of the simple and noble metals relative to the transition metals. But what about the optimal reaction path and the variation of forces as the molecule is rotated or translated away from this path, both significant in calculating the reaction rate under thermal conditions? The new developments¹⁻³ bear on these important details.

Cohen and colleagues¹ begin from the earlier discovery that the optimum path does not necessarily correspond to a molecular orientation and impact site such that the dissociation fragments are aimed at the locations where they will optimally reside on the surface. Specifically, calculations for a rhodium surface⁵ revealed that the favoured reaction path is asymmetric with respect to the surface lattice, with the H-atoms aimed at sites where they bridge two Rh-atoms. Only after the H_2 dissociates will the H-atoms move to the most favourable locations for chemisorbed atoms, the hollows marked 'h' in the figure. The 'obvious' dissociation route, shown in the lower part of the figure, is less favourable because it requires additional stretching of the relatively short H-H bond, at additional energy cost, before strong M-H bonds can form.

Whereas this conclusion was based on explicit energy and force calculations, Cohen *et al.* seek to develop an approximate theory based on the notion of a surface response function, a 'softness' or local electronic polarizability, which directly expresses the ease of promoting the looser metal electrons into strongly localized d -levels. To illustrate their approach, Cohen *et al.* show that a count of unfilled d -levels correlates with the optimal H_2 dissociation geometry found in ref. 5 for Rh(001). Although the predictive power of this softness function approach remains to be demonstrated, it could be a step on the path towards a 'frontier orbital' picture for surfaces^{6,7} that quantitatively correlates catalytic activity with clean surface attributes.

Direct calculations of molecular dissociation trajectories at surfaces have awaited accurate, fast computational methods for calculating forces. Accuracy is an issue because until recently no method was available that allowed absolute dissociation energies to be evaluated

adequately for systems of more than a few atoms. Speed is a concern because even H_2 -dissociation involves at least six degrees of freedom (three coordinates per H-atom, more if a thermal ensemble of metal lattice configurations is considered). The computational effort required obviously scales up with the dimension of the configuration space that must be explored.

Recent progress alleviates both problems. Density-functional calculations⁸, which have for years been used to predict accurate structures of molecules and solids, now incorporate corrections that allow evaluation of dissociation energies to a few kilocalories per mole (in many cases). At the same time, computing costs have dropped astonishingly. Inexpensive work stations and massively parallel computers make yesteryear's 'supercomputing' commonplace. This progress, together with methodological and algorithmic improvements (for example ref. 9), brings within the reach of first-principles calculations problems that only a decade ago were regarded as hopelessly inaccessible.

Simultaneous articles by Hammer *et al.*² and White *et al.*³ use modern hard- and software to arrive at the first detailed, global potential-energy surfaces for H_2 dissociation on a metal (Cu). Both calculations agree with the experimental conclusion that H_2 dissociation on Cu requires overcoming an energy barrier in the range of 0.5 to 1 eV. They also agree that this barrier is extremely corrugated along the Cu surface, and strongly dependent on molecular orientation.

Dynamical simulations of H_2 -Cu scattering processes remain to be carried out using the new potential-energy surfaces. When their results are compared to the many available experimental data on this system, we will know just how close we have come to having the important details of H_2 -dissociation in our grasp. In any event, the present series of papers promises a new era in the theory of surface chemical reactions. □

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Forever airborne

THE wandering albatross spends its time at sea, gliding over the crests and in the troughs of the waves. It seldom has to put power into its wings. Instead, it exploits the updraughts from wind streaming over the wave crests. It is, in fact, a flying machine powered by the interactions between waves and wind. In a flat calm, it has to rest on the water until active weather returns.

Daedalus wants to imitate this trick. He is designing an artificial albatross. It is essentially a fast-acting, variable-geometry glider. Tiny anemometers monitor the air currents flowing around it, and a small Doppler laser system scans the surrounding waves and their movements. An on-board computer processes these data and operates the control surfaces, so as to exploit those updraughts that permit the best progress in the programmed direction. Its systems will be powered by a small windmill rotor driven by its slipstream. It will be quite self-contained; over an active sea it will stay airborne indefinitely.

Much development work, both in hardware and software, will be needed to produce a working artificial albatross. It will never fly as gracefully as the real thing, but will share its limitations. In a flat calm, it too will have to come down onto the water. The subsequent take-off may be difficult. Daedalus plans to give the craft some sort of compressed-air jet device to punch it vertically aloft when the sea is active again. Once airborne, it will slowly recharge the jet reservoir with power bled from its windmill rotor, ready for the next ditching. In very rough weather, even real albatrosses sometimes get hit by waves, and have to recover from the blow and take off again from the churning water. This would be fatal for the artificial albatross. In a storm it will have to abandon its programmed course and simply keep as high as possible above the turbulent surface.

But with all these limitations, it will still be a wonderful oceanographic tool. Artificial albatrosses will quarter the oceans on tours of duty lasting months and spanning the globe. They will make close measurements of wave patterns, surface temperatures, oil slicks and so on, while satellites overhead track them and receive their findings, and relay fresh orders. Meteorologists will welcome their detailed accounts of remote wind and weather, navies will deploy them in antisubmarine warfare, and biologists will use them to shadow turtles and eels on their mysterious migrations. They might even be used to shadow real albatrosses, provoking interesting confrontations of rivalry or desire.

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