Quantum nutcracker for near-room-temperature hydrogen dissociation

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Catalytic molecular reactions or dissociations typically occur on crystal surfaces, but the most efficient materials are often very expensive. Nanoparticles are widely employed to both increase the surface area and reduce the cost. Here we provide the theoretical foundations for the design of a quantum nutcracker that exhibits efficient dissociation of hydrogen molecules. Each of the two nutcracker jaws, transition-metal phthalocyanine and a metal substrate such as Cu(111) or Au(111), is by itself inert for hydrogen dissociation. Density-functional-theory calculations demonstrate that, when a hydrogen molecule enters the channel between the jaws, it splits into two hydrogen atoms with high efficiency by quantum interactions and a gentle mechanical squeeze. Au-based nutcrackers are predicted to operate at room-temperature while less-expensive Cu-based ones are predicted to be active at a slightly elevated temperature. Indirect experimental evidence is consistent with the present predictions. Such in silico design holds promise for inexpensive, high-performance heterogeneous catalysts for H2 dissociation and may inspire new approaches to other complex reactions.

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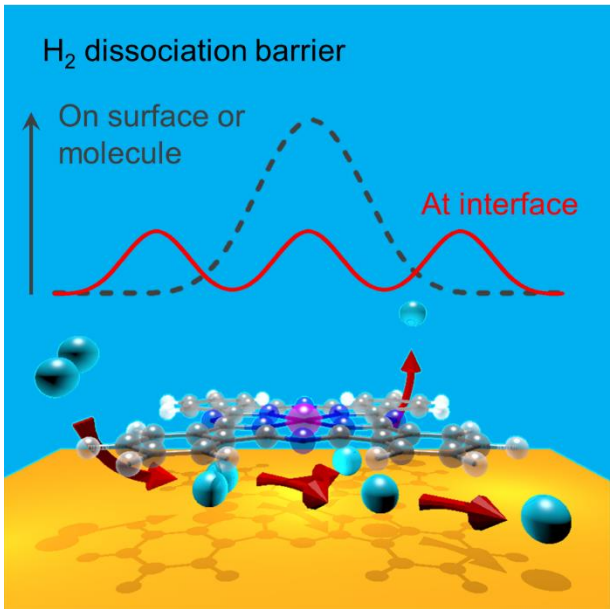

Schematics of H_2 dissociation at molecule/metal interface