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Spin-singlet resonance state in proton-embedded metals: A new paradigm for metallic screening to a point charge

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Hydrogen in metals has attracted attention for a long time from both basic scientific and technological points of view. Its electronic state has been investigated in terms of a proton embedded in the electron gas mostly by the local density approximation (LDA) to the density functional theory (DFT). At high electronic densities, it is well described by a bare proton H^+ screened by metallic electrons (charge resonance), while at low densities two electrons are localized at the proton site to form a closed-shell negative ion H^- protected from surrounding metallic electrons by the Pauli exclusion principle. However, no details are known about the transition from H^+ to H^- in the intermediate-density region. In this talk, the author shall explain its complete picture, in particular, a sharp transition from H^+ screening charge resonance to Kondo-like spin-singlet resonance, the emergence of which is confirmed by the presence of an anomalous Friedel oscillation characteristic to the Kondo singlet state through diffusion Monte Carlo (DMC) calculations with total electron number up to 170. This picture enriches the paradigm for metallic screening to a point charge with the addition of a possibility of spin resonance with a very long screening length, depending on the metallic density and the magnitude of charge. Besides, this work reveals that hydrogen is most stably embedded in the form of this spin-singlet resonance state, which may be important information for hydrogen storage in metals.

Biography

Yasutami Takada has completed his PhD on mechanisms of superconductivity in degenerate semiconductors from Tokyo University and Postdoctoral studies from Purdue University and University of California at Santa Barbara. In 1985, he joined in the division of Condensed Matter Theory, Institute for Solid State Physics, University of Tokyo as a faculty member and is now a Professor at the division concurrently with a Professor at Center of Computational Materials Science. He has published more than 110 papers in reputed journals and served as a Divisional Associate Editor of Physical Review Letters during 2001-2007.

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