4th International Symposium on
Energy Challenges & Mechanics
- working on small scales

11-13 August 2015
Aberdeen, Scotland, UK

New Route to Room-Temperature Superconductivity: Kondo Singlet State with T_K well beyond 1,000K in the Proton-Embedded Electron Gas

Yasutami Takada

Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan

Accepted for publication on 11th June 2015

Hydrogen in metals has attracted much 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. Here, by accurately determining the ground-state electron distribution $n(\boldsymbol{r})$ by the combination of LDA and diffusion Monte Carlo (DMC) simulations with the total electron number up to 170, we have obtained a complete picture of the transition, in particular, a sharp transition from H^+ screening charge resonance with a short screening length to Kondo-like spin-singlet resonance with a very long screening length, the emergence of which is confirmed by the presence of an anomalous Friedel oscillation characteristic to the Kondo singlet state with a Kondo temperature T_K well beyond 1,000K. This study not only reveals interesting competition between charge and spin resonances, enriching the century-old paradigm of metallic screening to a point charge, but also discovers a long-sought novel high-T_K system. Note that by referring to heavy-fermion physics, we may expect that superconductivity occurs at a temperature as high as $T_K/10$ (which is of the order of the room temperature) at an ambient pressure, contrary to the case of solid hydrogen or H_2S under very high pressures, if a macroscopic number of protons are embedded in a regular array into a metal in this intermediate-density region to synthesize a hydrogen alloy in the form of a periodic Kondo lattice.

Keywords: Kondo problem; Kondo singlet; hydrogen; heavy-fermion superconductivity.