Numerical modelling of hydrogen/deuterium absorption in transition-metal alloys

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Experimental investigation of anomalous heat effects from hydrogen isotope absorption in palladium lattice has proven to be an arduous task. Numerical modeling of the electronic structure of the Pd-H(D) system holds out the promise of identifying LENR active materials.

Multiple theories on hydrogen isotope fusion in Pd metal have been developed over the years. Among other important factors, the high concentration of H(D) atoms and their close proximity to each other within a host lattice are important. We use numerical modeling to investigate conditions favorable to lower H-H (D-D) separation. This separation depends on the background charge density within the lattice [1, 2]. Because of the high charge density in bulk Pd the internuclear distance between two hydrogen or deuterium atoms is larger than the value in vacuum [1]. However, the presence of lattice defects (vacancies [3], free-internal surfaces/cracks [4] and interstitials [5]) can lower the charge density down to the level which would promote the $H_2(D_2)$ molecule formation at closer separation.

We use the open-source software package QuantumEspresso to investigate $H_2(D_2)$ absorption in transition-metal alloys in the presence of different types of lattice defects and dopants. In addition to the previously reported effect of vacancies in Pd lattice [3], we find that doping the transition metals with elements of high electronegativity further lower the charge density and results in absorption of $H_2(D_2)$ with shorter separation distance.

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