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D-D (H-H) Interactions within the Interstices of Pd

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Abstract:

Embedded atom, local-density-functional, and Hartree-Fock methods are used to calculate the effective interaction between deuterium (or equivalently within the Born-Oppenheimer approximation hydrogen) nuclei within palladium. No effects were found to suggest that the repulsion between deuterons in gas phase D₂ is reduced within the octahedral and tetrahedral interstices of this transition metal.

Keywords:

palladium-deuterides, D₂, clusters, embedded atom method, density functional calculations, Hartree-Fock calculations, nuclear fusion