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First-principles simulations of transition metal ions in silicon as potential quantum bits[1] HE MA, The University of Chicago, Department of Chemistry and Institute for Molecular Engineering, HOSUNG SEO, The University of Chicago, Institute for Molecular Engineering, GIULIA GALLI, The University of Chicago, Institute for Molecular Engineering and Argonne National Laboratory
— Optically active spin defects in semiconductors have gained increasing attention in recent years for use as potential solid-state quantum bits (or qubits). Examples include the nitrogen-vacancy center in diamond, transition metal impurities, and rare earth ions. In this talk, we present first-principles theoretical results on group 6 transition metal ion (Chromium, Molybdenum and Tungsten) impurities in silicon, and we investigate their potential use as qubits. We used density functional theory (DFT) to calculate defect formation energies and we found that transition metal ions have lower formation energies at interstitial than substitutional sites. We also computed the electronic structure of the defects with particular attention to the position of the defect energy levels with respect to the silicon band edges. Based on our results, we will discuss the possibility of implementing qubits in silicon using group 6 transition metal ions.

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