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Surface magnetic susceptibility of silicon nanoclusters from machine learning electronic structure

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Abstract

Silicon nanoclusters, as intermediate structures between molecules and bulk silicon, provide a unique platform for studying size-dependent transitions in structural, electronic, and magnetic properties. In contrast to bulk crystalline silicon, which is weakly diamagnetic, silicon clusters may exhibit a temperature-dependent paramagnetic response and interesting behavior due to dominant surface effects, quantum confinement, surface reconstruction, and the dangling bonds. Being highly sensitive to the density of electronic states near the Fermi level, accurate determination of the Fermi level plays a key role in predicting magnetic susceptibility. We present a computational framework in which atom-projected density of states is predicted using machine learning, while a local chemical potential is assigned to each atom based on the equilibrium charge distribution. By combining these two ingredients, we obtain a single-particle approximation of the magnetic susceptibility of individual atoms. For pure silicon nanoclusters, we show that the contribution of surface atoms to the magnetic response is significantly larger than that of interior atoms. The overall magnetic susceptibility of the particle decreases with increasing nanocluster diameter and approaches the bulk value. This result is consistent with the general behavior of nanoparticles and merits further experimental investigation or the development of models that go beyond the present framework by incorporating spin interactions and exchange (Stoner) enhancement.

Keywords: Silicon clusters, Magnetic susceptibility, Local density of states, Machine learning.

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