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Multiscale study of artificial quantum lattices formed on Cu(111) surfaces using CO molecules

Artificial lattices of carbon monoxide (CO) molecules on Cu(111) surfaces serve as powerful platforms for probing topological quantum effects relevant to quantum information science (QIS). In this multiscale computational study, we integrate density functional theory (DFT) and density functional tight-binding (DFTB) to characterize the electronic properties of honeycomb and Kagome CO lattices. Accurate DFT calculations of CO adsorption energetics and charge distributions validate and calibrate our DFTB parameterizations. Leveraging DFTB, we then simulate extended lattices, systematically varying molecular spacing and adsorption registries to assess their impact on surface density of states, band structure, and charge-transfer phenomena. Our results demonstrate that fine-tuning lattice parameters can markedly alter the electronic landscape and coherence properties of these artificial systems. These atomistic insights establish clear structure–property relationships and provide critical guidance for experimental efforts to develop robust, tunable CO-based platforms for next-generation QIS technologies.

Topical Area

Hard matter: quantum, electronic, semiconducting materials

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