Metal Adatoms at 2D Materials: Structure, Reactivity and Magnetic Properties

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Using density functional theory (DFT), we studied microscopic mechanisms governing adsorption, initial stages of the growth, reactivity, and magnetic properties of selected metal nanostructures on two-dimensional (2D) materials. For metals on graphene, we found the tendency of alkaline and alkaline-earth atoms towards 2D growth, while transition metal atoms form three-dimensional structures [1]. Structural defects can be utilized to prevent the clustering of transition metal adatoms and to stabilize them in the form of monomers [2]. These adatoms are examples of single-atom catalysts with promising properties regarding hydrogen adsorption and recombination [2]. Graphene on Ni(100) forms a striped moiré pattern, enabling selective adsorption of metal atoms and small clusters. Our DFT calculations reveal electrostatic interaction as the origin of preference of Au to bind on the valleys and Co to adsorb at the ridges, as confirmed in recent experiments [3].
Using borophene on Ag(100) as a substrate, we investigated 2D magnetic nanostructures formed by the adsorption of Fe atoms. Combining DFT with the anisotropic Heisenberg model and Monte Carlo simulations, we estimate the critical temperatures of 105 K and 30 K for the Fe-based magnets grown above or under borophene, respectively [4].

References

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