First-principles Study on the Kondo Resonance in a Two-Dimensional Ni-HHTP on Au(111)

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Two-dimensional metal-organic frameworks (MOFs) have emerged as promising candidates for quantum spin liquids and qubits due to their tunable self-assembly into distinct patterns. In this study, we report a theoretical investigation of the Ni-HHTP (2,3,6,7,10,11-hexahydroxytriphenylene) complex on Au(111). Using density functional theory (DFT), we analyzed the electronic structure and oxidation states of Ni at various adsorption sites, exploring the effect of Ni-substrate interaction. Additionally, we identified magnetic moments of the Ni centers due to unpaired electrons, which could explain the Kondo resonance in the system. These findings provide valuable insights into spin interactions in 2D MOFs and highlight their potential for quantum computing and spintronics platforms.