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Dynamics of tungsten and cobalt carbonyls on silica surfaces
KALIAPPAN MUTHUKUMAR, ROSER VALENTI, HARALD O. JESCHKE, Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — Metal carbonyl species adsorbed on a substrate are the starting point for the electron beam induced deposition of metallic nanostructures. We employ first principles molecular dynamics simulations to investigate the dynamics of tungsten hexa- and pentacarbonyl as well as cobalt octacarbonyl precursor molecules on fully and partially hydroxylated silica substrates. We find that physisorbed carbonyls are quite mobile on a silica surface saturated with hydroxy groups, moving around half an Angstrom per picosecond. In contrast, chemisorbed ions like $[W(CO)_5]^-$ or $[Co(CO)_4]^-$ are more stable at room temperature. We determine the vibrational spectra which can provide signatures for experimentally distinguishing the form in which precursors cover a substrate.

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