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**Interaction of $W(CO)_6$ with $SiO_2$ Surfaces** JUAN SHEN, KALIAPPAN MUTHUKUMAR, HARALD O. JESCHKE, ROSER VALENTI, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt Germany — The interaction of tungsten hexacarbonyl $W(CO)_6$ precursor molecules with $SiO_2$ substrates is investigated by means of density functional theory calculations with and without inclusion of long range van der Waals interactions. We consider two different surface models, a fully hydroxylated and a partially hydroxylated $SiO_2$ surface, corresponding to substrates under different experimental conditions. For the fully hydroxylated surface we observe only a weak interaction between the precursor molecule and the substrate with physisorption of $W(CO)_6$. Inclusion of van der Waals corrections results in a stabilization of the molecules on this surface. In contrast, we find a spontaneous dissociation of the precursor molecule on the partially hydroxylated $SiO_2$ surface where chemisorption of a $W(CO)_5$ fragment is observed upon removal of one of the CO ligands from the precursor molecule. Irrespective of the hydroxylation, the precursor molecule prefers binding of more than one of its CO ligands. In the light of these results, implications for the initial growth stage of tungsten nano-deposits on $SiO_2$ in an electron beam induced deposition process are discussed. [1] K. Muthukumar et al. Phys. Rev. B (in press) (2011)

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