

Abstract Submitted
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Substrate Mediated Short-range and Long-range Adsorption Pattern of CO on Ag(110)¹ WAI-LEUNG YIM YIM, Institute of High Performance Computing, Singapore, THORSTEN KLUENER, Institute for Pure and Applied Chemistry, Theoretical Chemistry, University of Oldenburg, Germany — Substrate-mediated intermolecular interactions were proposed in the literature to explain the adsorption of CO on Ag(110) but the underlying mechanism is yet to be known. Here, short-range and long-range relaxation patterns for CO adsorption on Ag(110) surfaces have been investigated. The relaxation mode can be explained by the interaction of heavy electrons on metal substrates in electron momentum space. We identified two relaxation modes for CO on Ag(110). The long-range relaxation involved a (6×6) commensurate phase, while the short-range relaxation involved an alleviation of Fermi surface nesting along the $\langle 1\bar{1}0 \rangle$ direction of the Ag(110) substrate. The symmetry broken ground state structure at high CO coverage can be rationalized, and this structure is consistent with the interpretation of available experimental data.

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