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Molecular Dynamics Simulation of Adsorption of Methane and Chloromethane on Molybdenum via Hybrid EAM/OPLS Interactions[1]

GARY LEUTY, MESFIN TSIGE, Department of Polymer Science, The University of Akron — The question of liquid adsorption on the surface of a solid substrate has been of major interest to computational science even from its inception. Accurate depictions of adsorption phenomena require accurate modeling of both phases of the simulated system. In cases in which accuracy of the models leads to the adoption of potentially inconvenient or incompatible force fields, questions arise as to whether joint systems can perform as well as needed to gather optimal data. The current investigation uses molecular dynamics (MD) tools to focus, in part, on how well-developed models for liquid simulation (OPLS, built on a Lennard-Jones foundation) can combine with tested models for metals (based on functionals of electron density) to describe the adsorption of methane and chloromethane on the surface of molybdenum. Comparisons have been made between the differences in effect of a hybrid EAM/OPLS system and systems focusing solely on Lennard-Jones-based interactions, as well as the effect of large asymmetry and polarity differences in adsorbate species, on the structure and dynamics of layers adsorbed directly at the surface of the metal substrate. Preliminary results suggest that the surface landscape and corrugation play a significant role in choice of surface binding sites.

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