

Quantitative Determination of Organic-Metal Interactions with Molecular Dynamics Simulations in Revolutionary Accuracy and Speed

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Interface Force Field (IFF) is a CHARMM-based force field database for life science and materials discovery using molecular dynamics (MD) simulations. The developed IFF contains the models and parameters of metals, ions, oxides, gases, polymers, minerals and 2D materials, and is validated as a highly reliable and accurate tool to theoretically research the interfacial interactions and energies. We employ an example system with benzene/naphthalene molecules adsorbed on Pt(111) surface to precisely calculate the heat of adsorption. The breakthrough herein is the concept of introducing virtual pi electrons for the aromatic rings to simulate the impacts of pi electron clouds in reality. With the new IFF model and parameters, a revolutionary accuracy of 100% is achieved for the heat of adsorption determination for both benzene and naphthalene molecules, which is distinctly superior to CHARMM-IFF and density-functional theory (DFT). Moreover, with the comparison with perfect Pt(111) surface, it is discovered that concave defects on Pt(111) surface turn out larger heat of adsorption while large terraces and islands leads to similar heat of adsorption estimation. This work offers referential and reliable models and force field parameters that can be used for quantitative prediction/determination of organic-metal interfaces, which is of great significance in the applications such as material science, catalysis, biological engineering and pharmaceutical molecules.

Biography

Cheng Zhu obtained his Ph.D from Soochow University and is now conducting postdoctoral studies at Department of Chemical and Biological Engineering, University of Colorado Boulder. He has published more than 35 papers (2 journal covers) in reputed journals and has been serving as editorial board members of Journal of Biotech Research & Biochemistry and Journal of Protein Research & Bioinformatics. He was awarded the National scholarship for doctoral students (2017), the Suzhou industrial park scholarship (2019), and the outstanding dissertation of Soochow University (2020).

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