



中国科学院
Research Laboratory for
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学术报告(2013-6-17)

题目: van der Waals 力起主导作用的分子-电极界面原子尺度结构

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摘要:

Van der Waals (vdW) interaction plays a fundamental role in fields as diverse as supramolecular chemistry, structural biology, polymer science, surface science, and condensed matter physics. On the experimental side, in 2012, first direct measurements of the strength of vdW force for molecule/metal interfaces were made by two groups, via atomic force microscopy (AFM). On the theory side, vdW density functionals (vdW-DF) are proposed and now, especially for the optimized versions of vdW-DF, can treat physisorbed systems in a relative accurate and fast way. This presentation will report our recently works on the role of vdW interaction in interface atomic structures determining for molecules adsorbed on surfaces and for molecule-electrode interfaces.

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