Fitting empirical force fields for Co-Salen on NaCl

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The self-assembly of metal-organic molecules Salen ((Co(C16H14N2O2)) on the bulk NaCl(100) surface, has been measured using non-contact atomic force microscopy. These room temperature measurements, observe two different morphologies, a metastable nanowire and a stable nanocrystallite [1]. To investigate how these structures form and their reasons for their relative stabilities, an approach using empirical force fields is required, due to the size of the computational model required. However, no parametrisation of a force field exists in the literature that is able to describe the three interaction regimes required; Intermolecular, intramolecular and molecule-surface interactions. A common issue in fitting force fields for this type of systems is the lack of suitable reference experimental data, hence the force field will be fitted to ab initio Density Functional Theory (DFT) calculations. Due to the large number of coefficients in the force field, the parameter space is huge and an indirect approach to sample and optimise the force field is required. In this work, an genetic algorithm (GA) [2] has been used to optimise the force field to describe the intramolecular and molecule-surface interactions. The resulting GA optimised force field has then been tested against both experimental and theoretical results, that were not part of the fitting set, such as adsorption energy and adsorption geometry.

References:

[1] S. Fremy, *et al*,Nanotechnology, vol. 20, no. 40, p. 405608, 2009.

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