Study of reliability of aluminium cluster models for the description of chemisorption

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Cluster models of chemisorption are widely used to interpret experimental observations in surface science. In recent calculations on chemisorption on aluminium surfaces we have become aware that commonly used models for Al surfaces suffer from a major weakness in that the Al clusters used have very high electron affinities, at least in DFT calculations. A theoretical result in sharp contrast to the experimental observation.

In order to understand this result and its consequences for studies of chemisorption better we have studied the electron affinities and ionization potentials of Al clusters at higher levels of quantum chemical calculation. We performed CCSD(T) calculation employing Dunning's correlation consistent basis sets cc-PVxZ of Al clusters of different sizes.