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Development of Neural-Network Potentials for Atomistic Modelling of PWI

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Artificial neural-networks (NN) have been used to model the potential-energy surfaces of, for example, bulk silicon or copper surfaces. NNs may reach the structural and energetic quality of density-functional theory (DFT) at a small computational cost [1][2]. The authors intend to develop NN potentials based on ab initio data as an alternative approach to empirical potentials for the atomistic modeling of plasma wall interaction processes (PWI).
At the stage of the 'training'process, we obtain data for Be-W surfaces and small molecular clusters of BenWm, BenHm, WnHm with $n + m \leq 4$ including also the pure species with $m = 0$.

In the present contribution, we focus on a comparison of quantum chemical methods for BenWm, BenHm, WnHm species. Second order perturbation theory (MP2) and coupled cluster CCSD(T) theory are compared with plane-wave and atomic orbital DFT calculations, and with available experimental data. The plane-wave calculations were carried out with the VASP code using the PBE functional for the description of exchange and correlation of valance electrons, and the projector augmented wave approximation for inner shell electrons. The atomic orbital calculations have been performed with the Gaussian code, where we employ the double hybrid B2PLYD3 and the dispersion corrected ωB97X-D functional and also compare the performance of various ECP basis sets. With preliminary results and the knowledge from literature, we can already conclude that a single method will probably not be sufficient to deal with molecular clusters and surfaces alike.

[1] Jorg Behler and Michele Parrinello, PRL 98, 146401 (2007)
[2] Nongnuch A., Behler J, PHYSICAL REVIEW B 85, 045439 (2012)

Eligible for student paper award?

Yes

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