Be/W/H containing molecules near surfaces: Data-driven approach for fast and accurate calculations of their properties

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Hot plasma in contact with a solid wall can sputter atoms from it, leading in fusion applications to unwanted degradations of wall compounds. The sputtered atoms can react with other ones to create a layer of small molecules that cannot be neglected in the overall energy balance. We created a small data base of such fusion-relevant molecules consisting of the elements tungsten, beryllium and hydrogen and others. Their properties were calculated via CCSD(T) with the intent to find out how the much cheaper density functional methods compare with the high-level method [1]. Despite obtaining some guidelines, no single density functional was satisfactorily reproducing all the properties (geometry, atomization energy and so on). We applied a relatively new method of statistical learning (Lasso, [2]) to check the performance of linear and nonlinear combinations of density functionals. Even a linear combination of two or three density functionals can reproduce the CCSD(T) properties (fig.1).

Figure 1. Left: DFT energies compared to CCSD(T); Right: Performance of a combined functional for bond lengths (red) and energies (blue).


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