Data accuracy in modelling and computation: Some examples

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In this poster we give two examples from our work on plasma-wall interaction – related topics. The first example about the computation of electron-impact cross sections (EICS). It is an example where even large errors do not make the computations useless.
A typical electron-impact cross section, calculated in two different ways, looks like this:
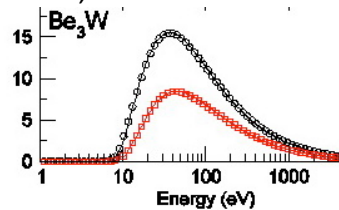
The reality is believed to lie between the two curves which are, however, still the best ways of approximate the cross section. The main reason why the result is not useless is that the EICS is often the end-product or that it can be relatively easily checked if using the black or the blue curve influences the results of plasma simulations. What can we make better ?

The second example deals with the quantum mechanical calculations on the stability, expressed as cohesive energies, of Be-W alloys, a potentially important plasma facing material:

structure	E_{coh} [eV/atom]		Literature data
	DFT	ABOP	
Be hcp	3.727	3.32	3.7[a], 3.32[b]
W bcc	8.485	8.89	8.53[c], 9.010[d]
			8.66[e], 8.90[b]
Be$_2$W	5.591	6.96	7.037[f]
Be$_{12}$W	4.190	4.86	3.12[a]

Here we see very typical deviations which, are cumbersome because they can make the difference between erosion and persistence. Because their reasons are multidimensional, error bars are also not meaningful - they would be too large although the modelling is sound. What can one make better in this case ?

We end with some thoughts (compiled by KH and modified by MP) from a symposium in Uppsala, June 2014 that dealt with a similar topic as the present workshop.
Some questions:
1. Who should actually perform the modelling – only experts to whom everything is outsourced? Or non-experts and experimentalists too ?
2. What – if anything – is desirable to do about the plethora of atomistic force-fields that are used within the scientific community and amongst the end-users ? The same question concerning software and method "with similar functionality".
3. Do presently really exist many, or even any, application areas where the materials

models and modelling techniques are currently good enough to consistently provide predictable results and insights for (industrial) end-users ?

Some answers:
- What is needed is usually not numbers, but rather chemical or physical insight, relations, and rules of thumb, in order to help in the processes of ranking and performance predictions. T*his is good news because modelling is often better in insights than in exact numbers. But it often means that the numbers are not yet within reach.*
- The quality (accuracy, transferability, ...) of currently available atomistic interaction models - force fields and so on - is often **not** sufficient to extract observables in a reliable way (i.e. within desired error limits). In a multi-scale framework, such shortcomings will carry over to the levels "above", as the information is transferred to more coarse-grained models.
    What can we make better again ?

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