Краткая аннотация лекции

«The Inexhaustible Rise of Materials Computer Simulation»

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Our understanding of materials performance is based on experimental data. We use it to inform predictive models that allow us to develop better materials and sometimes even new materials. Experimental data is, however, often challenging to obtain either because the controlling factor takes place on time scales or length scales that are challenging or the systems themselves are hazardous, especially nuclear materials. In these circumstances computer simulations can be exceptionally useful.

We use the results of simulation in four different ways: to provide property values for existing models and understand experimental values; to ‘check’ or ‘test’ existing assumptions; to improve existing models by ‘developing’ the physical models; or sometimes even to develop totally new models, using the simulations to ‘discover’ or ‘identify’ the physics/chemistry behind the process.

In this seminar we will consider each of these in turn, to see how high performance computing can add value to the development of materials.