Speaker: **Tobias Binninger, Theory and Computation of Energy Materials (IEK-13), Institute of Energy and Climate Research, Forschungszentrum Jülich)**

Title: **Quantum annealing methods for optimization problems in energy materials research**

Date: **Monday, June 24, 15:00 pm**

Place: **Seminar room 915**

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Abstract:

Quantum computing technologies are expected to strongly impact computational research in materials science in the future. With the emergence of real quantum computing hardware, it is of great interest to identify and demonstrate challenging research problems where quantum computing can provide new solutions. Modeling of ionic arrangements in multielements compounds represents a ubiquitous challenge for computational research in energy materials. Materials with mixed or partially occupied lattice sites are widely investigated, e.g.,doped semiconductors for photovoltaics, or intercalation materials for Li-ion batteries. While the configurational arrangement of elements greatly impacts the materials' properties, construction of reliable models of occupation disorder represents a major difficulty for simulations. The exponential scaling of the configuration space renders the search for the configurational ground state a classically hard-to-solve problem. In this seminar talk, I will introduce an optimization method that enables the use of quantum annealing (QA) to determine the ionic ground state configuration in a battery material [1]. The method relies on a grand-canonical transformation of the energy cost function that strongly reduces the effective coupling strengths of the interaction graph, which is essential for effectiveness of quantum annealing. The optimization results and sampling statistics obtained on a D-Wave Advantage quantum annealer will be discussed. I will finally provide an outlook how we envisage extending the approach to circuit-based quantum optimization in the future.

[1] T. Binninger, Y.-Y. Ting, P. M. Kowalski, M. H. Eikerling, arXiv:2401.02165