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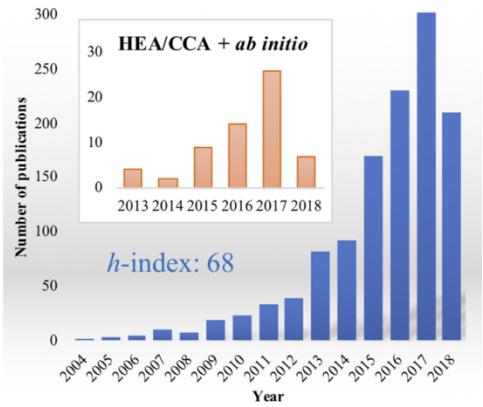
Research topics:
Computational materials science
Ab initio thermodynamics
Magnetism
High entropy alloys and steels
Phase stability and chemical ordering

Complex Concentrated Alloys

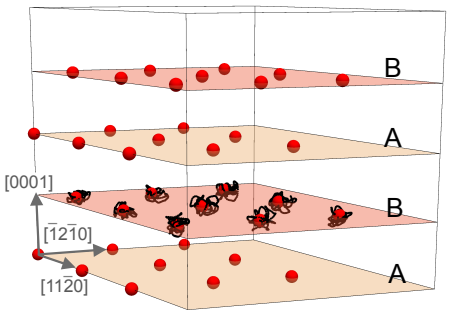
The key focus of the Complex Concentrated Alloys' (CCA) group is to develop the computational tools to satisfy the ongoing and increasing demands for the computational design and data-driven exploration of complex, multi-component alloys including the recent class of high entropy alloys (HEAs). HEAs have attracted remarkable attention since their discovery 2004 due to their various excellent materials properties and the sheer endless possibilities to explore new alloys. The alloys are mostly investigated by experiments, but ab initio calculations have emerged as a powerful approach that complements experiment and can serve as a predictive tool to explore materials properties of new promising alloys. To achieve this goal the CCA group focuses in particular on advancing the current state-of-the-art ab initio approaches towards complex multi-component alloys.



*Published articles on HEAs and CCAs until mid- 2018. Inset: Works including ab initio calculations. [*Ikeda, Grabowski, Körmann, Mater. Charact. (2018)].

A particular important quantity is the stacking fault energy (SFE), which has significant impact on the deformation and mechanical properties of materials. The temperature dependence of the SFE for most elements has remained experimentally inaccessible due to technical difficulties. In [Zhang et al., PRB 2018] we perform highly-accurate ab initio calculations to investigate the temperature dependence of the SFE for three prototypical elements Al, Cu, and Ni and compare with an extensive set of previous theoretical and experimental data. Our results clearly reveal a strong and unexpected reduction of the SFE with temperature and clarify the contribution of the different excitation mechanisms.

The CCA group is currently advancing these computational tools towards multicomponent alloys.



Sketch of ab initio MD trajectories in a hcp cell (with ABAB… stacking). Such calculations have been employed in [Zhang et al., PRB 2018] to compute highly-accurate finite-temperature SFEs from ab initio.

Key publications 2018:

Zhang et al., Phys. Rev. B, in press (2018)
Stockem et al., Phys. Rev. Lett. 121, 125902 (2018)
Ikeda et al., Mater. Charact. (2018)
Gong et al., Phys. Rev. B 97, 214106 (2018)
Ikeda et al., npj Comput. Mater 4, 7 (2018)
Dutta et al. PSS B 255, 1700455 (2018).
Ikeda et al., Entropy 20, 655 (2018)