



INTERDISCIPLINARY CENTRE FOR  
ADVANCED MATERIALS SIMULATION

## ICAMS Seminar

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ICAMS Seminar Room 0.08

### Phase stability and dislocation shear resistance of the $\gamma'$ phase of Co-Al-W-based alloys

The discovery of a  $\gamma+\gamma'$  two-phase field in the Co-Al-W ternary phase diagram has led to a strong interest in new  $\gamma'$ -strengthened Co-based superalloys. Thanks to their outstanding creep properties and low solute segregation during solidification, these alloys may be apt to substitute Ni-based superalloys in the hot stages of gas turbines. Beside their value in industrial applications, Co-based superalloys also present a number of opportunities from a scientific perspective. Electronic- and atomic-scale modeling methods can be adopted to develop these alloys using a bottom-up approach. Moreover, their Ni-based relatives can serve as a reference to highlight differences and similarities between the two distinct alloys systems. The use of electronic- and atomic-scale modeling methods also presents a number of challenges, mainly linked to their current limitations with system size (number of atoms that can be simulated) and the inclusion of entropic effects (simulations at finite temperatures). This talk focuses on how first-principle simulations may provide valuable insights on phase stability and mechanical properties – both important to alloy design.

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