INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Wednesday, 11 September, 3:30 p.m.
Room IC 02-718

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Molecular simulations you can trust and reproduce: The OpenKIM framework

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The quality of classical molecular and multiscale simulations hinges on the suitability of the employed interatomic model (IM) for a given application. Reproducibility of simulations depends on the ability of researchers to retrieve the original IM that was used. These two issues are addressed by the Open Knowledgebase of Interatomic Models project (https://openkim.org). OpenKIM curates IMs with full provenance control, issues them DOIs so that they can be cited in publications, and tests them exhaustively using "KIM Tests" that compute a host of material properties and "Verification Checks" on coding correctness. OpenKIM is integrated into major simulation packages (including ASE, DL_POLY, GULP and LAMMPS) allowing users to easily use OpenKIM IMs and query their predictions. Machine learning based tools for selecting an IM and assessing uncertainty are under development. OpenKIM functionality provides major benefits to researchers and promises to improve the reliability and reproducibility of molecular simulations of materials.