



The European Materials Modelling Council

Project idea presentation

- DT-NMBP-09-2018: Accelerating the uptake of materials modelling software (IA)
- Main Contact:
 - Fraunhofer Institute for Algorithms and Scientific Computing SCAI
 - Jan Hamaekers, Department Virtual Materials Design
<jan.hamaekers@scai.fraunhofer.de>
 - Mission: Development of innovative methods in the field of Computational Science, including their implementation and the provision of products for the industrial take-up
 - Unique feature: products and projects
 - Several (numerical) software products
(e.g. multiphysics/coupling, atomistic modelling, optimization, solvers)



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- Contact: Fraunhofer SCAI, Jan Hamaekers: <jan.hamaekers@scai.fraunhofer.de>
- Topic: **Electrochemical Energy Converters**
- Objectives:
 - Integrate software for electrochemical modelling (all scales)
 - Focus on batteries and fuel cells
 - Provide top-down and bottom-up design and remove model complexities for end-user
- ML, Data Analysis, Reduced Order Models, Multiscale Modelling
- Expected results: Unique software environment: TRL 7
- Partners:
 - Modelling (discrete: QM, MM/MD, ...; continuum: PNP, ...)
 - Software vendors
 - End users