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This course was also taught as part of the Singapore-MIT Alliance (SMA) programme as course number SMA 5107 (Atomistic Computer Modeling of Materials).

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Atomistic- and Multiscale Modeling of Materials Failure Christian Thaulow, Dept Engineering Design and Materials, NTNU, Norway. All knowing depends on the structure of the knower We do not see that we do not see Material optimization process. Fracture Mechanics. Historical Development. 1 000 000 000 000 000 000 From LARGE Scale testing: 100MN and 10 minutes to Atomistic Mechanics: 10pN and 1

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Atomistic modeling is used in an increasing number of projects, either to supplement information from TCAD modeling (band structure, material parameters) or in its own right, to better understand material properties and material interfaces (defects, etc.).

Forschungszentrum Jülich - Atomistic Modelling

The aim of our atomistic modeling studies is to use the powerful supercomputing resources located at Forschungszentrum Jülich and allied institutions to perform virtual experiments that reveal crucial information on the atomic-scale mechanisms that govern the interactions of radionuclides with various materials, including those constituting the storage and disposal environments.