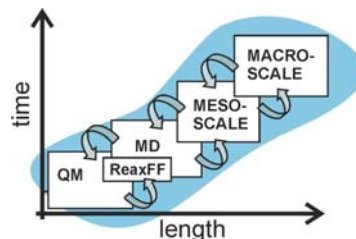


# 1<sup>st</sup> Workshop on Multi-Paradigm Multi-Scale Modeling in the Computational Materials Design Facility (CMDf)



**Tuesday, Aug. 23 & Wednesday, Aug. 24, 2005**  
Materials and Process Simulation Center (MSC),  
California Institute of Technology, Pasadena, CA



**Workshop organizers:** Dr. Markus Buehler (MSC), Prof. Dr. William Goddard III (MSC)

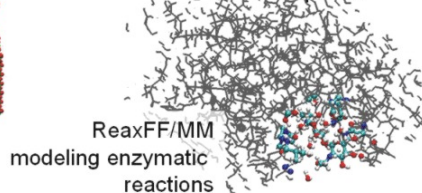
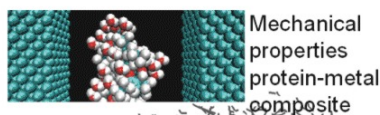
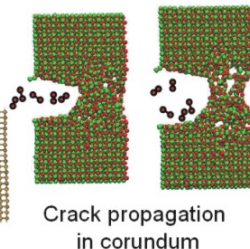
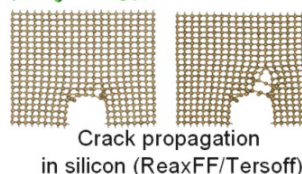
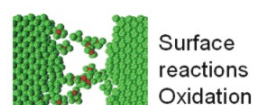
**Topic and motivation:** Provide a forum for discussions around multi-scale multi-paradigm modeling activities. Particular focus will be on MSC's newly developed CMDf framework (funded by DARPA-PROM) and the Materials Properties Facility (funded by ASC). We hope to stimulate discussion on various related topics and approaches in multi-scale and multi-paradigm modeling.

**Website:** <http://www.wag.caltech.edu/home/mbuehler/cmdf/>

**Confirmation and participation:** Please register at <http://winpc1.wag.caltech.edu/>

**Program (tentative): Tuesday, Aug. 23**

William A. Goddard III	Introduction to MSC
Markus Buehler	Introduction and Overview: Multi-scale multi-paradigm modeling
Rick Muller	Historical perspective on Python and scientific computing
Jef Dodson	Extended OpenBabel: CMDf's central data structure
Hatem Helal	Quantum mechanical modeling within the CMDf and applications to modeling of low energy electron enhanced etching LE4
Adri van Duin	Reactive force fields: A new link from QM to MM
Paul van Allmen (JPL)	Thermoelectric properties and sensitivity analysis
Daniel Yi	Time acceleration methods in CMDf: The Temperature Accelerated Dynamics method (TAD) coupled with ReaxFF
Li Tao	Coupling of ReaxFF and DREIDING for hybrid modeling of biological systems and reactions in enzymes
Victor Kam	The CMDf SCREAM method for proteins
Alberto Cuitino	Bridging to the continuum scale
Vaidehi Nagarajan	Bio-applications of CMDf
Frank Ducheneaux	Implicit solvation methods for discrete systems
Barry Olafson	The Molscape GUI module for CMDf
Julius Su	ElexFF: A new electron force field
Si-ping Han	Reactive force fields ReaxFF and metal-oxide systems



**Wednesday,  
Aug. 24**

**Training sessions:**  
Hands-on training  
sessions on CMDf  
usage will be held  
(BI subbasement,  
please register).  
Assisted by the

CMDf developers, we will train interested scientists how to set up and perform simulations.