DOE Symposium on New Theoretical Concepts and Directions in Catalysis, University of California, Santa Barbara
noon, Tuesday August 27 through noon, Friday August 30, 2013
Elings Hall 1601
http://catalysis.cnsi.ucsb.edu/

TUESDAY, AUGUST 27, 2013

start	**end**	
I: session chair = Horia Metiu		
1:30 pm	2:30	Matthias Scheffler, ñThermodynamics and statistical mechanics from first principles for surfaces and interfaces: Theoretical challenges, concepts, and insightsò
2:30	3:30	Roger Rousseau, ñ*Ab initio* molecular dynamics for computational catalysisò
3:30	*4:00*	*break*
4:00	5:00	Michael Janik, ñDensity functional theory methods for examining active sites of M-doped ceria surfacesò
5:00	6:00 pm	Mark Gordon, ñStrategies for studying catalysis using accurate quantum chemistryò

WEDNESDAY, AUGUST 28, 2013

start	**end**	
II: session chair = Matthias Scheffler		
8:30 am	9:30	Horia Metiu, ñCatalysis by modified oxides: How to use DFTò
9:30	10:30	Baron Peters, ñIsolated catalyst sites on amorphous supports: a systematic *ab initio* algorithm for dispersive kineticsò
10:30	*11:00*	*break*
11:00	noon	Gustavo E. Scuseria, ñProjected Hartree-Fock theory: a low cost alternative to multi-reference wavefunction methodsò
noon	*1:30 pm*	*lunch*
III: session chair = Baron Peters		
1:30 pm	2:30	John C. Tully, ñNonadiabatic chemistry at surfacesò
2:30	3:30	Priya Vashishta, ñReactive nanosystems: Multimillion to billion atom Molecular Dynamics simulationsò
3:30	*4:00*	*break*
4:00	5:00	Keiji Morokuma, ñAutomatic exploration of potential energy surfaces for catalysis and other complex chemical reactionsò
5:00	6:00 pm	Karsten Reuter, ñFirst-principles microkinetic modeling of surface catalytic reactions: reality and visionsò

THURSDAY, AUGUST 29

start	**end**	
IV: session chair = John Tully		
8:30 am	9:30	Jens Nørskov (presented by Horia Metiu), ñIn search of the catalyst genomeò
9:30	10:30	Garnet Chan, ñFrom bioinorganic catalysts to the solid stateò
10:30	*11:00*	*break*
11:00	noon	Discussion with industrial scientists
noon	*1:30 pm*	*lunch*
V: session chair = Michael Janik		
1:30 pm	2:30	Martin Head-Gordon, ñSome recent advances in density functional theory methods and algorithms with implications for catalysis modelingò
2:30	3:30	Filipp Furche, ñAccurate barrier heights from renormalized RPA perturbation theoryò
3:30	*4:00*	*break*
4:00	5:00	Zhipan Liu, ñThe stochastic surface walking method and its application in catalysisò
5:00	6:00 pm	Dionisios G. Vlachos, ñCombinatorial complexity, uncertainty, and emergent behavior in the design of catalytic materialsò

FRIDAY, AUGUST 30

start	**end**	
VI: session chair = Dion Vlachos		
8:30 am	9:30	Troy Van Voorhis, ñCharge transfer and catalysis at the nanoscale: Really big molecules or really small solids?ò
9:30	10:30	Michel Dupuis, ñModeling molecular and interfacial processes in molecular electrocatalysis and in photocatalysis: Successes and challengesò
10:30	*11:00*	*break*
11:00 am	noon	Wrap-up discussion
noon	*1:30 pm*	*lunch*