Telluride Workshop: “Computational Materials Chemistry” Agenda

Telluride Intermediate School, 725 W Colorado Ave, Telluride, Colorado

Tuesday, June 23, 2015 morning to Saturday, June 27, 2015 noon; Breakfast 7:45am-8:30am at School

Tuesday June 23, 2015

8:20am-8:30am opening remarks

Session I: Structure prediction; Chair: Richard Hennig

8:30am-9:20am Yanming Ma (Jilin Univ.): Materials Discovery via CALYPSO Methodology

9:20am-10:10am Eva Zureck (SUNY Buffalo)

10:10am-10:40am Coffee Break

10:40m-11:30am David Wales (Cambridge)

11:30am-12:20am De-en Jiang (UCR): First principles structure prediction for metal clusters

Wednesday June 24, 2015

Session II: Materials in catalysis and energy; Chair: De-en Jiang

8:30am-9:20am Thomas Bligaard: SLAC, Stanford

9:20am-10:10am Jeff Greeley (Purdue)

10:10am-10:40am Coffee Break

10:40am-11:30am Graeme Henkelman (UT Austin)

11:30am-12:20pm Maria Chan (Argonne)

6pm-9pm (estimate): Telluride Posters and Picnic in honor of R. Stephen Berry

Thursday June 25, 2015

Session III: Surfaces, interfaces, and organic materials; Chair: Donald Siegel

8:30am-9:20am Yong-Kyun Kim (KAIST): “*Ab Initio* Surface Chemistry of Colloidal Quantum Dots”

9:20am-10:10am Tomas Arias (Cornell): “Joint Density-Functional Theory: pathway to fully rigorous and computationally efficacious ab initio electrochemistry”

10:10am-10:40am Coffee Break

10:40am-11:30am Qin Wu (BNL): “Organic electronic materials”

11:30am-12:00pm Greg Beran (UCR): “High accuracy chemical shielding predictions in molecular crystals for NMR crystallography”

Friday June 26, 2015

Session IV: 2D Materials; Chair: Jeff Greeley

8:30am-9:20am Hongjun Xiang (Fudan): “Global Structure Prediction of Two Dimensional Materials"

9:20am-10:10am Zhongfang Chen (UPR): 2D materials

10:10am-10:40am Coffee Break

10:40am-11:30am Richard Hennig (U. Florida)

11:30am-11:55pm Benjamin Revard (Cornell)

Saturday June 27, 2015

Session V: Simulating materials properties; Chair: Graeme Henkelman

8:30am-9:20am Donald Siegel (Michigan): “Discovery of MOFs for CO2 capture and energy storage”

9:20am-10:10am Xinqgqiu Chen (IMR, CAS): “Elastic Deformation with Topo. Phase Transition in Na3Bi”

10:10am-10:40am Coffee Break

10:40am-11:05am Logan Ward (Northwestern)

11:05am-11:30am Penghao Xiao (UT-Austin)

11:30am-11:45pm Concluding remarks