

Version – Aug. 11, 2017 – Final as presented

Telluride Workshop: “Computational Materials Chemistry” Agenda
Telluride Intermediate School, 725 W Colorado Ave, Telluride, CO 81435
Monday, Aug. 7, 2017 morning to Friday noon, Aug. 11; Breakfast 7:30am-8:30am at School

Monday, 7 Aug 2017

8:20am-8:30am opening remarks

Session I: 2D materials beyond graphene; Chair: De-en Jiang/Don Siegel

8:30am-9:20am David Tomanek (MSU): Low-dimensional semiconductors beyond graphene

9:20am-10:10am Hai-Ping Cheng (UF): Interface and transport of few-layer vertical tunneling junctions

10:10am-10:40am Coffee Break

10:40am-11:30am Wolfgang Windl (OSU): 2D-Materials beyond Graphene

11:30am-12:20am Richard Hennig (UF): Magnetic 2D materials for spintronics applications

Tuesday, 8 Aug 2017

Session II: 2D and ultrathin materials in catalysis; Chair: Graeme Henkelman/Greg Beran

8:30am-9:20am Yujie Sun (USU): Biomass valorization coupled with hydrogen production via 2D catalysts

9:20am-10:10am Aleks Vojvodic (UPenn): Layered and 2D Transition Metal Compounds as Electrocatalysts

10:10am-10:40am Coffee Break

10:40am-11:30am Jeff Greeley (Purdue): Catalysis at quasi-1D and -2D metal/oxide interfaces

11:30am-12:20pm De-en Jiang (UCR): Chemical functionalization of 2D materials and electrocatalysis

Wednesday, 9 Aug 2017

Session III: 2D materials: chemical properties and charge storage; MOFs; Chair: Aleks Vojvodic/Jianwei Sun

8:30am-9:20am Talat Rahman (UCF): Chemical activity of 2D materials: defect-laden MoS₂ and h-BN

9:20am-10:10am Brandon Wood (LLNL): Quantum effects governing charge storage in 2D materials

10:10am-10:40am Group Photo and Coffee Break

10:40am-11:30am Don Siegel (Michigan): Computational Discovery of MOFs

11:30am-12:05pm Peilin Liao (Purdue): Optimizing open Fe sites in MOFs for ethane oxidation

Thursday, 10 Aug 2017

Session IV: Catalysis; Student/Postdoc Talks; Chair: Yujie Sun/Richard Hennig

8:30am-9:10 am Aaron Holder (CU Boulder): Predicting metastable phases

9:10am-10:00am Graeme Henkelman (UT Austin): ZPE, transition state theory, and reaction rate

10:00am-10:10am Jeff Greeley (Purdue): Clarification of some issues

10:10am-10:40am Coffee Break

10:40am-11:00am Dan Liu (MSU): Vibrational modes in quasi-2D and quasi-1D structures

11:00am-11:20am Joshua Paul (UF): 2D Material Discovery and Photocathode Application

11:20am-11:40am Zhibin Gao (Tongji/MSU): 2D SiO₂ with in-Plane Negative Poisson's Ratio

11:40am-12:00pm Yubo Zhang (Tulane): Ferroelectric systems with the SCAN meta-GGA

Friday, 11 Aug 2017

Session V: Molecular crystal, solid, and meso systems; student talks; Chair: David Tomanek/Hai-Ping Cheng

8:30am-9:20am Greg Beran (UCR): Ab Initio Molecular Crystallography: Aiding & Abetting Experiment

9:20am-10:10am Jianwei Sun (Tulane): SCAN density functional

10:10am-10:45am Chun-wei Pao (Academia Sinica): Mesoscale morphology of organic solar cells

10:45am-11:15am Coffee Break

11:15am-11:35am Christopher Bartel (CU Boulder): Machine learning of inorganic solids

11:35am-11:55am Samantha Millican (CU Boulder): Design of Piezoelectric heterostructural alloys

11:55am-12:00pm Concluding remarks