Talks at APS 2021 March Meeting by participants in USAfrI
By Richard Martin

The USAfrI workshop is the day before the main meeting on Sunday March 14 at 8AM to noon. See the program at http://usafricainitiative.org/APS2021/

Here is a list of talks by USAfrI Speakers during the main meeting (Monday - Friday)
28 Total (there may be more I did not find)

You can find talks by each person by searching using the author index at the website http://meetings.aps.org/Meeting/MAR21/Content/3990.
(Also many of the talks are listed in posters at the USAfrI workshop.)

Tunna Baruah - several talks - some on DFT theory
Stanimir Bonev - two talks - high pressure
Maria Chan - **Invited talk** plus many others - Machine learning, data ...
Valentino Cooper, several talks - computational design
Michel Cote - ML phonons, ….
Robert Distasio - **Invited talk** + other talks
Elif Ertekin - **invited talk**
Marco Fornari - several talks
Giulia Galli - **Invited talk** plus many others
Marco Govoni - many talks - Simulations , using quantum computers
Sinead Griffin - many talks
Vladimir Mujica Y13.00010 Intrinsic Rashba coupling due to hydrogen bonding in DNA and Oligopeptid
Marco Buongiorno Nardelli - several talks - various - using quantum computers
Rina Pandey C54.00002 Freestanding Sr2IrO4 nanomembranes: structural and optical properties
Mark Pederson - several talks - some on DFT theory
Yuan Ping - many talks
John Rehr - several talks
Brenda Rubenstein F21.00011 Finite Temperature Auxiliary Field Quantum Monte Carlo in the Canonical Ensemble
Sashi Satpathy M36.00012 Orbital and Spin Hall effect: Effect of symmetry breaking and Density-Functional results for MoS2
James Shepherd - three talks
Andre Schleife - **Invited talk** - several other talks - Dynamics - TDDFT
Mehmet Topsakal Y61.00005 Machine-Learning X-Ray Absorption Spectra to Quantitative Accuracy-
David Vanderbilt - many talks
Lucas Wagner - several talks related tp QMC
Cai-Zhuang Wang - many talks
Renata Wentzcovitch - many talks - coauthor of an invited talk
Chris Wolverton **- Invited talk** plus several other talks related to Machine Learning computational discovery
Houlong Zhuang, C57.00005 Disordered hyperuniform networks and their application in atomic-scale low-dimensional materials

Invited Talks by USAfrl people

A60.00001: Network Theory Meets Materials Science

Invited Speaker: Christopher Wolverton

One of the holy grails of materials science, unlocking structure-property relationships, has largely been pursued via bottom-up investigations of how the arrangement of atoms and interatomic bonding in a material determine its macroscopic behavior. Here we consider a complementary approach, a top-down study of the organizational structure of networks of materials, based on the interaction between materials themselves. We demonstrate the utility of applying network theory to materials science in two applications: First, we unravel the complete “phase stability network of all inorganic materials” as a densely-connected complex network of 21,000 thermodynamically stable compounds (nodes) interlinked by 41 million tie-lines (edges) defining their two-phase equilibria, as computed by high-throughput density functional theory. Using the connectivity of nodes in this phase stability network, we derive a rational, data-driven metric for material reactivity, the “nobility index”, and quantitatively identify the noblest materials in nature. Second, we apply network theory to the problem of synthesizability of inorganic materials, a grand challenge for accelerating their discovery using computations. We use machine-learning of our network to predict the likelihood that hypothetical, computer generated materials will be amenable to successful experimental synthesis. *** In collaboration with V. Hegde, M. Aykol, S. Kirklin, L. Hung, S. Suram, P. Herring, and J. Hummelshoj*

E60.00001: Capturing and Leveraging Computational and Experimental Data in Materials Physics

Invited Speaker: Maria Chan

In order to use artificial intelligence and machine learning for scientific advances, access to complex, multimodal, and accurate data is critical. In this talk, we will discuss efforts in generating, capturing, and leveraging computational and experimental data, with examples in generation of computational defect properties datasets, capturing microscopy data, and combining streams of computational and experimental data. We will also discuss concerted efforts at US Department of Energy Scientific User Facilities in data infrastructure.

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F19.00001: Towards an Accurate and Efficient Order-*N* Framework for Real-Space Condensed-Phase Hybrid Density Functional Theory

Invited Speaker: Robert Distasio

By including a fraction of exact exchange (EXX), hybrid functionals reduce the self-interaction error in semi-local density functional theory (DFT), and thereby furnish a more accurate and reliable description of the electronic structure in systems throughout chemistry, physics, and materials science. However, the high computational cost associated with hybrid DFT limits its applicability when treating large-scale and complex condensed-phase systems. To overcome this limitation, we have devised a highly accurate and linear-scaling (order-N) approach based on a local (MLWF) representation of the occupied space that exploits sparsity when evaluating the EXX interaction in real space [1]. In this work, we present a detailed description of the theoretical and algorithmic advances that are needed to perform hybrid DFT based ab initio molecular dynamics (AIMD) simulations of large-scale finite-gap condensed-phase systems using

this approach. This is followed by a critical assessment of the accuracy and parallel performance of the exx algorithm when performing AIMD simulations of liquid water and several ice phases in the canonical (NVT) and isobaric-isothermal (NpT) ensembles. With access to high-performance computing (HPC) resources, we demonstrate that exx enables hybrid DFT based AIMD simulations of systems containing 500-1000 atoms with a wall time cost comparable to semi-local DFT. In the strong-scaling limit, this cost is split evenly between computation, communication, and processor idling; as such, we also discuss a three-pronged strategy that directly attacks each of these contributions and reduces the overall wall time cost by approximately an order of magnitude for large-scale heterogeneous systems. With these developments, this work takes us one step closer to routinely performing AIMD simulations of large-scale condensed-phase systems for sufficiently long timescales at the hybrid DFT level.

[1] J Chem Theory Comput 16, 3757 (2020).

J53.00001: Defect Chemistry and Dopability of Telluride Diamond-Like Semiconductors and Ordered Vacancy Compounds for Thermoelectric Applications

Invited Speaker: Elif Ertekin

Computation-driven search for candidate thermoelectric materials has recently resulted in several successes, but many of the predicted materials often prove to be difficult to dope in the lab. This presentation will review our recent computational and experimental efforts to tailor and understand defect chemistry and dopabaility of a chemically-diverse set of telluride-based diamond-like semiconductors (DLS) of interest for their potential as thermoelectrics. We consider the I_BIIITe$_2$ with I_B=(Cu,Ag), III=(In,Ga) and Cu$_2$(Zn,Cd,Hg)(Si,Ge,Sn)Te$_4$ material space, and use first-principles methods and experimental phase boundary mapping to comprehensively assess dopabilities in this search space. These materials are typically observed to be p-type, but a materials descriptor suggests that they would be more effective as thermoelectrics if they could be doped n-type. Therefore, we comprehensively establish the achievable range of carrier concentrations using calculations of phase stability, defect formation energies, and carrier concentrations. Using phase boundary mapping, experimental carrier concentrations are measured and compared to the predicted values, showing a correspondance within a few orders of magnitude. For all compounds, a delicate competition between I_{III}, III$_I$, and V_I defects governs the achievable range of carrier concentrations -- and enhancing n-type behavior requires suppressing the I_{III} and V_I defects while enhancing the III$_I$ antisites. Using this observation as a design strategy, we identify candidate diamond like semiconductors that may be more amenable to n-type doping. The results of this comprehensive search are used to generate a chemically intuitive framework for predicting dopabilities in this family of materials without the need to carry out full-scale first-principles analysis.

L22.00001: Electron and ion dynamics in materials after particle radiation and optical excitation

Invited Speaker: Andre Schleife

Quantum states of matter are tied to the interplay of interactions in the Hamiltonian and novel states can emerge in materials depending on the relative coupling strength, e.g. between electronic and lattice degrees of freedom as well as coupling to external fields. Fabricating and processing novel materials for electronic devices with nanoscale dimensions requires extremely precise techniques with control at the atomic level. In addition, characterizing and probing properties, e.g. via electronic and optical excitations, require knowledge about a material on ultrafast time scales. In this talk I will present recent quantum-mechanical first-principles predictions for electron dynamics and the

subsequent ionic motion that follows after an initial excitation of the electronic system in semiconductors and metals. In particular, we showed that long-lived electronic excitations in proton irradiated MgO can facilitate diffusion of oxygen vacancies. For silicon material under swift heavy ion irradiation, we analyzed the charge state dynamics of the projectile ion and used it to explain electronic stopping behavior. Finally, for proton and laser irradiated aluminum surfaces, we quantify electron emission, projectile charge capture, and pre-equilibrium electronic stopping behavior, that is unique to thin films and two-dimensional materials. Limitations an

P18.00005: Electronic structure and coherence properties of spin defects in two-and three-dimensional semiconductors from first principles

Invited Speaker: Giulia Galli

We report on recent progress in investigating the electronic structure [1] and coherence properties [2] of spin defects in three- and two-dimensional materials using first principles electronic structure calculations (DFT and many body perturbation theory), and spin Hamiltonians [3]. In particular we present results for defects in SiC, and MoS_2.

[1] H. Ma, M. Govoni and G. Galli, npj, Comput. Mat., 6 (85), (2020)
[2] A. Bourassa et al., Nat. Mat. 2020; M. Onizhuk et al. arXiv. 2020. 2010.11077; M. Ye, H. Seo and G. Galli, npj Comp. Mat. 5 (44), 1-6 (2019)
[3] K. Ghosh, H. Ma, V. Gavini and G. Galli, Phys. Rev. Mat. 3, 043801 (2019).

V20.00001: Thermal Conductivity of $CaSiO_3$ Perovskite at Lower Mantle Conditions

Invited Speaker: Zhen Zhang

Renata is coauthor

Thermal conductivity (κ) of mantle minerals modulates strongly both the style of mantle convection and the time scale of the Earth's mantle and core cooling. It is therefore a fundamental parameter for geodynamic modeling. Cubic $CaSiO_3$ perovskite (cCaPv) is believed to be the third most abundant mineral in the lower mantle (LM) (7 vol%). However, despite its importance, investigations of its properties are challenging because of its strong anharmonicity. cCaPv is dynamically unstable at low temperatures and its phonon spectrum has imaginary frequencies from harmonic phonon calculation. Particularly for κ, prevailing theoretical approaches such as perturbative methods encounter difficulties in dealing with such strong anharmonicity. Experimental measurements at relevant high pressures and temperatures are equally challenging. Therefore, no previous estimate of cCaPv's κ exists at mantle conditions, experimental or theoretical. Here we present *ab initio* quantum mechanical results of this property obtained using an established phonon quasiparticle approach that can address the strongly anharmonic situation in cCaPv. These results are substantiated by direct experimental measurements of this property at LM conditions. These results and data agree very well and reveal a surprisingly large κ of cCaPv compared to $MgSiO_3$-perovskite, which is only weakly anharmonic.

Y22.00001: Cumulant Green's function methods for excited state properties of functional materials

Invited Speaker: John Rehr

Many interesting properties of functional materials depend on their excited state properties, such as dynamic response and thermodynamic behavior. Often this behavior depends on details of excitations in the system such as phonons and plasmons, which lead to inelastic losses and damping effects. These

excitations can be probed by photoemission spectra, where they show up as satellites beyond the quasi-particle peak [1]. These many-body effects are neither amenable to density functional theory nor extensions based on quasi-particle approximations. Here we discuss an approach based on the cumulant Green's function, which provides a unified treatment of such dynamic correlation effects [2]. The approach is illustrated with several applications. Remarkably, a cumulant calculated in linear response within a quasi-boson approximation, is adequate to explain the loss spectra and charge-transfer excitations in many systems. Finite-temperature exchange-correlation potentials, thermodynamic properties, and the finite-temperatureTDDFT kernel, and can also be obtained [3,4]. Finally, some extensions are briefly discussed, including nonlinear contributions to the cumulant [5].

[1] Jianqiang Sky Zhou et al., PNAS, https://doi.org/10.1073/pnas.2012625117.
[2] L. Hedin, J. Phys.: Condens. Matter 11, R489 (1999).
[3] J. J. Kas, et al., Phys. Rev. B 100, 195144 (2019).
[4] John J. Rehr and Joshua J. Kas, Eur. Phys. J. B 91, 153 (2018).
[5] M. Tzavala et al., Phys. Rev. Research 2, 033147 (2020).