

APS March Meeting 2016 – Baltimore, MD

- **G. Galli**

- H32.00001 [Predicting materials for solar energy conversion: ab-initio spectroscopy of heterogeneous interfaces](#)
- H32.00012 [Photoemission spectra of aqueous solutions of salts from many-body perturbation theory](#)
- C20.00007 [Solvated ions as defects in liquid water: A first-principles perspective](#)
- C32.00004 [Probing the interface between semiconducting nanocrystals and molecular metal chalcogenide surface ligands: insights from first principles](#)
- H32.00013 [Coupled experimental and theoretical study of photon absorption and charge transport in BiVO₄ photoanodes for solar water splitting](#)
- F24.00003 [First Principles Simulations of Nanoparticle Solids](#)
- B20.00004 [Dielectric-dependent Density Functionals for Accurate Electronic Structure Calculations of Molecules and Solids](#)
- B51.00012 [Atomistic simulations of activated processes in nanoparticle synthesis](#)
- H54.00008 [A joint \emph{first principles} and ATR-IR study of the vibrational properties of interfacial water at semiconductor-water solid-liquid interfaces](#)
- K21.00001 [Ab initio Raman spectroscopy of water under extreme conditions](#)
- K21.00004 [Dissolved carbon in extreme conditions characterized by first principles simulations](#)
- K33.00008 [Electronic structure properties as signatures of morphological motifs in organic photovoltaics](#)
- K52.00001 [Ligand engineering of lead chalcogenide nanoparticle solar cells](#)
- H31.00013 [A non-empirical, parameter-free, hybrid functional for accurate calculations of optoelectronic properties of finite systems](#)
- V7.00007 [Isolation of dangling bond states on Si\(100\) surfaces for quantum information applications](#)
- Y5.00001 [Microscopic origin of the prolonged coherence in 4H-SiC divacancy spin qubits](#)

- **J. J. de Pablo**

- X37.00001 [Topological defects in liquid crystals as templates for molecular self-assembly.](#)
- B53.00013 [Simulations of high and low viscosity micro-scale droplets splashing on a dry surface](#)
- F33.00002 [A particle-in-mesh method for Brownian Dynamics simulation of many-particle systems with hydrodynamics interactions in a confined geometry](#)
- A35.00005 [Active nematics confined within a shell](#)
- P22.00005 [Accurate, efficient, and scalable parallel simulation of mesoscale electrostatic/magnetostatic problems accelerated by a fast multipole method.](#)
- R33.00008 [Surprising increase in photostability of organic amorphous materials by efficient molecular packing](#)
- P36.00001 [Directed self-assembly of colloidal particles onto the chemically anchoring patterned surface in a nematic liquid crystal](#)
- P36.00003 [Directed Self-assembly of Colloidal Particles on a Blue Phase I Interface](#)
- X37.00002 [Molecular nature of liquid crystal defects](#)
- X37.00003 [\textbf{Topological defects and self-assembly of cuboidal colloidal particles with sharp edges in a nematic liquid crystal}.](#)
- S37.00009 [\textbf{Structural organization of liquid crystals at liquid crystal-air interface: Synchrotron X-ray reflectivity and computational simulations}](#)
- R39.00010 [The role of Nucleosome Positions on Chromatin Structure: A multi-scale approach](#)
- M1.00211 [Colloidal particles embedded in liquid crystal droplets](#)
- P36.00010 [Tactoids of chiral liquid crystals](#)

- **F. Gygi**

- B20.00012 [Data compression algorithms for electronic wave functions](#)
H54.00008 [A joint \emph{first principles} and ATR-IR study of the vibrational properties of interfacial water at semiconductor-water solid-liquid interfaces](#)
P14.00003 [The Road to Interoperable Simulation Software: Examples Using the Qbox Code](#)

- **J. Mitchell**

- A26.00005 [Isotropic and anisotropic regimes of the spin-dynamics in \$\text{Sr}_2\text{IrO}_4\$: Field-dependent Raman scattering study](#)
Y6.00007 [Single crystal preparation and long-range charge fluctuations in the square-planar nickelate \$\text{La}_4\text{Ni}_3\text{O}_8\$.](#)
F31.00005 [ARPES Study of Triple Layer Nickelate \$\text{R}_4\text{Ni}_3\text{O}_{10}\$ \(R=Pr, La\)](#)

- **D. Awschalom**

- Y5.00001 [Microscopic origin of the prolonged coherence in 4H-SiC divacancy spin qubits](#)
H7.00012 [Optimizing the Growth of \(111\) Diamond for Diamond Based Magnetometry](#)
H45.00011 [Restoring photon indistinguishability via pulse and continuous-wave control of solid-state quantum emitters.](#)
K12.00010 [Optical Control of Ferromagnetism in a Magnetically-Doped Topological Insulator](#)
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V45.00004 [Robustness of optically-controlled Berry phase in a diamond spin qubit](#)
Y5.00013 [Optical and Spin Signatures of Transition Metal Impurities in Silicon Carbide](#)

- **M. K. Chan**

- H32.00007 [First principles investigations on the stability and catalytic reactivity of \$\text{Cu}_2\text{O}\$ surfaces](#)
L31.00007 [Joint Density Functional Theory for the electrode/electrolyte interface: Benchmarking liquid structure with experiment and \it ab initio molecular dynamics](#)
L23.00001 [Computational design and optimization of energy materials](#)
X7.00005 [First principles modeling of grain boundaries in CdTe](#)

- **L. Curtiss**

- H54.00002 [The Basic Understanding of Lithium Superoxide in \$\text{Li-O}_2\$ Battery](#)

- **M. Olvera de la Cruz**

- H37.00009 [Multiscale simulations of nanoribbon structures from chromophore amphiphile self-assemblies](#)
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A33.00012 [Morphology-induced low temperature conductivity in ionic liquids.](#)
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C33.00002 [Energy conversion in polyelectrolyte hydrogels](#)

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E37.00003 [Novel liquid crystal phase transition of linear defects in an epitaxial layer of DNA-nanoparticle superlattices](#)

H34.00002 [Driving magnetic colloidal polymers](#)

- **P. Fenter**

H17.00011 [Spatially Correlated Disorder in Epitaxial van der Waals Heterostructures](#)

L31.00007 [Joint Density Functional Theory for the electrode/electrolyte interface: Benchmarking liquid structure with experiment and *ab initio* molecular dynamics](#)

- **S. C. Glotzer**

A36.00014 [Controlling Chirality of Entropic Crystals](#)

E36.00001 [Fluid to solid transition of hard regular polygons](#)

E36.00004 [Digital Alchemy for Materials Design: Colloids and Beyond](#)

E36.00005 [Shaping Crystal-Crystal Phase Transitions](#)

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H37.00001 [Implicit depletion of anisotropic particles](#)

K37.00011 [Clusters of polyhedra in spherical confinement](#)

A34.00004 [Electric-field mediated propulsion in binary colloidal suspensions](#)

E37.00010 [The role of symmetry for the orientational ordering of hard regular polygons](#)

- **O. Heinonen**

V18.00011 [Observation of room-temperature skyrmion Hall effect.](#)

V24.00002 [The effect of Ta "oxygen scavenger layer" on HfO₂-based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport](#)

X18.00009 [Generation of magnetic skyrmion bubbles by inhomogeneous spin-Hall currents](#)

L5.00007 [Spin wave band structure of artificial square ices](#)

L6.00003 [Theory of mode coupling in spin torque oscillators coupled to a thermal bath of magnons](#)

P22.00005 [Accurate, efficient, and scalable parallel simulation of mesoscale electrostatic/magnetostatic problems accelerated by a fast multipole method.](#)

R19.00011 [A Study of Phase Stability and Properties of TiO₂ Polymorphs with Diffusion Monte Carlo](#)

- **M. G. Kanatzidis**

P11.00012 [Cs vacancy ordering and properties of phase separated Cs_xFe_{2-y}Se₂](#)

V11.00004 [Spectroscopic evidence for temperature dependent relative movement of light and heavy hole valence bands of PbQ \(Q=Te,Se,S\)](#)

E11.00005 [Studying the morphology of the magnetic C₄ phase in the 122 superconductors.](#)

E11.00006 [Itinerant Double-Q Spin-Density Wave in Iron Arsenide Superconductors](#)

E28.00004 [Probing the Superconducting Proximity Effect of Topological Insulator \$\text{Bi}_2\text{Se}_3\$ Using Scanning Tunneling Microscopy](#)

L17.00012 [Mapping of the photo-induced metastable and hidden phases in 2D electronic materials](#)

X7.00008 [Electronic structure and defect properties of selenophosphate](#)

[Pb₂PS₆Se₆ for \$\gamma\$ -ray detection¹](#)

V11.00001 [James C. McGroddy Prize for New Materials Talk: From discovery to design of new materials](#)

- **D. Talapin**

C32.00004 [Probing the interface between semiconducting nanocrystals and molecular metal chalcogenide surface ligands: insights from first principles](#)

- **J. Whitmer**

A33.00004 [Explicit-ion Effects in the Coil-Globule Transition of Weak Polyelectrolytes](#)

H37.00010 [Self-assembly of Ionic Chromonic Liquid Crystals](#)

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