

Jan.

1. Density functional theory is straying from the path toward the exact functional

<http://science.sciencemag.org/content/355/6320/49>

2. What every physicist should know about string theory, *Physics Today* 68 (2015) no.11, 38-43.

<http://physicstoday.scitation.org/doi/pdf/10.1063/PT.3.2980>

Feb.

1. Synthesis of Freestanding Graphene on SiC by a Rapid-Cooling Technique

<http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.117.205501>

2. Observation of the Wigner-Huntington transition to metallic hydrogen

<http://science.sciencemag.org/content/early/2017/01/25/science.aal1579>

3. Discrete Time Crystals: Rigidity, Criticality, and Realizations,

<http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.118.030401>

4. Solving the quantum many-body problem with artificial neural networks

<http://science.sciencemag.org/content/355/6325/602.full>

Mar.

1. Efficient generation of generalized Monkhorst-Pack grids through the use of informatics

<http://journals.aps.org/prb/abstract/10.1103/PhysRevB.93.155109>

2. Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed

<http://pubs.acs.org/doi/abs/10.1021/ct800531s>

3. Different Ways of Hydrogen Bonding in Water - Why Does Warm Water Freeze Faster than Cold Water?

<http://pubs.acs.org/doi/abs/10.1021/acs.jctc.6b00735>

4. Multiconfiguration Pair-Density Functional Theory

<http://pubs.acs.org/doi/full/10.1021/ct500483t>

Apr.

1. Formamide reaction network in gas phase and solution via a unified theoretical approach: Toward a reconciliation of different prebiotic scenarios

<http://www.pnas.org/content/112/49/15030>

2. Battle between quantum and thermodynamic laws heats up

<http://www.nature.com/news/battle-between-quantum-and-thermodynamic-laws-heats-up-1.21720>

May.

1. A general derivation and quantification of the third law of thermodynamics

<https://www.nature.com/articles/ncomms14538>

2. Quantum vertex model for reversible classical computing

<https://www.nature.com/articles/ncomms15303>

3. Artificial gravity field, astrophysical analogues, and topological phase transitions in strained topological semimetals

<http://www.nature.com/articles/s41535-017-0026-7>

4. Single-crystal Ih ice surfaces unveil connection between macroscopic and molecular structure

<http://www.pnas.org/content/114/21/5349>

June.

1. Towards accurate quantum simulations of large systems with small computers
<https://www.nature.com/articles/srep41263>
2. Holy Grails for Computational Organic Chemistry and Biochemistry
<http://pubs.acs.org/doi/abs/10.1021/acs.accounts.6b00532>
3. Negative-Mass Hydrodynamics in a Spin-Orbit-Coupled Bose-Einstein Condensate
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.118.155301>

July.

1. Satellite-based entanglement distribution over 1200 kilometers
<http://science.sciencemag.org/content/356/6343/1140>
2. Simplifying the representation of complex free-energy landscapes using sketch-map
<http://www.pnas.org/content/108/32/13023.abstract>
3. Extracting Crystal Chemistry from Amorphous Carbon Structures
<http://onlinelibrary.wiley.com/doi/10.1002/cphc.201700151/full>

August.

1. A Theoretical Challenge: Transition-Metal Compounds
<http://www.ingentaconnect.com/content/scs/chimia/2009/00000063/00000003/art00008>
2. Intrinsic map dynamics exploration for uncharted effective free-energy landscapes
<http://www.pnas.org/content/114/28/E5494>
3. Diffusive dynamics during the high-to-low density transition in amorphous ice
<http://www.pnas.org/content/114/31/8193.abstract.html?etoc>

September.

1. The Elephant in the Room of Density Functional Theory Calculations
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcllett.7b00255>
2. Simulating Chemical Kinetics Without Differential Equations: A Quantitative Theory Based on Chemical Pathways
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcllett.7b01760>
3. Energy Ordering of Molecular Orbitals
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcllett.6b02517>
with comments <http://pubs.acs.org/doi/abs/10.1021/acs.jpca.7b05789>
4. Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets
<http://www.nature.com/nature/journal/v549/n7671/full/nature23879.html>

October.

1. A Study on the Coffee Spilling Phenomena in the Low Impulse Regime
<http://www.sciencedirect.com/science/article/pii/S2078152015300377>
2. On the Rheology of Cats
http://www.rheology.org/sor/publications/rheology_b/RB2014Jul.pdf
3. Exact Factorization of the Time-Dependent Electron-Nuclear Wave Function
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.105.123002>
4. Assessing Density Functionals Using Many Body Theory for Hybrid Perovskites
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.119.145501>

November.

1. Importance of σ Bonding Electrons for the Accurate Description of Electron Correlation in Graphene
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.119.166402>
2. Automatic chemical design using a data-driven continuous representation of molecules
<https://arxiv.org/pdf/1610.02415.pdf>

3. Complexity Reduction in Large Quantum Systems: Fragment Identification and Population Analysis via a Local Optimized Minimal Basis
<http://pubs.acs.org/doi/abs/10.1021/acs.jctc.7b00291>
4. Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.117.115702>

December.

1. Nuclear Quantum Effects in Water Reorientation and Hydrogen-Bond Dynamics
<http://pubs.acs.org/doi/abs/10.1021/acs.jpcclett.7b00979>
2. Discovery and Characterization of a Pourbaix-Stable, 1.8 eV Direct Gap Bismuth Manganate Photoanode
<http://pubs.acs.org/doi/abs/10.1021/acs.chemmater.7b03591>