

Property Correlations and Predictions

Adsorption of CO on Low-Energy, Low-Symmetry Pt Nanoparticles: Energy Decomposition Analysis and Prediction via Machine-Learning Models

Raymond Gasper, Hongbo Shi, and Ashwin Ramasubramaniam

The Journal of Physical Chemistry C **2017** 121 (10), 5612-5619

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Machine Learning Approach for Prediction and Understanding of Glass-Forming Ability

Y. T. Sun, H. Y. Bai, M. Z. Li, and W. H. Wang

The Journal of Physical Chemistry Letters **2017** 8 (14), 3434-3439

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Genetic Optimization of Training Sets for Improved Machine Learning Models of Molecular Properties

Nicholas J. Browning, Raghunathan Ramakrishnan, O. Anatole von Lilienfeld, and Ursula Roethlisberger

The Journal of Physical Chemistry Letters **2017** 8 (7), 1351-1359

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Intrinsic Bond Energies from a Bonds-in-Molecules Neural Network

Kun Yao, John E. Herr, Seth N. Brown, and John Parkhill

The Journal of Physical Chemistry Letters **2017** 8 (12), 2689-2694

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Introducing a New Potential Figure of Merit for Evaluating Microstructure Stability in Photovoltaic Polymer-Fullerene Blends

José Darío Perea, Stefan Langner, Michael Salvador, Benjamin Sanchez-Lengeling, Ning Li, Chaohong Zhang, Gabor Jarvas, Janos Kontos, Andras Dallos, Alán Aspuru-Guzik, and Christoph J. Brabec

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Resolving Transition Metal Chemical Space: Feature Selection for Machine Learning and Structure–Property Relationships

Jon Paul Janet and Heather J. Kulik

The Journal of Physical Chemistry A **2017** 121 (46), 8939-8954

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Extrapolating Energetics on Clusters and Single-Crystal Surfaces to Nanoparticles by Machine-Learning Scheme

Ryosuke Jinnouchi, Hirohito Hirata, and Ryoji Asahi

The Journal of Physical Chemistry C **2017** 121 (47), 26397-26405

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Predicting Catalytic Activity of Nanoparticles by a DFT-Aided Machine-Learning Algorithm

Ryosuke Jinnouchi and Ryoji Asahi

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Materials Discovery

Designing High Dielectric Permittivity Material in Barium Titanate

Jinghui Gao, Yongbin Liu, Yan Wang, Xinghao Hu, Wenbo Yan, Xiaoqin Ke, Lisheng Zhong, Yuting He, and Xiaobing Ren

The Journal of Physical Chemistry C **2017** 121 (24), 13106-13113

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Machine Learning Assisted Predictions of Intrinsic Dielectric Breakdown Strength of ABX₃ Perovskites

Chiho Kim, Ghanshyam Pilania, and Rampi Ramprasad

The Journal of Physical Chemistry C **2016** 120 (27), 14575-14580

DOI: <http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b05068>

Forcefields and potential energy surfaces

Modeling Segregation on AuPd(111) Surfaces with Density Functional Theory and Monte Carlo Simulations

Jacob R. Boes and John R. Kitchin

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Machine Learning Force Fields: Construction, Validation, and Outlook

V. Botu, R. Batra, J. Chapman, and R. Ramprasad

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Representing Global Reactive Potential Energy Surfaces Using Gaussian Processes

Brian Kolb, Paul Marshall, Bin Zhao, Bin Jiang, and Hua Guo
The Journal of Physical Chemistry A **2017** 121 (13), 2552-2557
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Proton-Transfer Mechanisms at the Water–ZnO Interface: The Role of Presolvation

Vanessa Quaranta, Matti Hellström, and Jörg Behler
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DOI: <http://pubs.acs.org/doi/abs/10.1021/acs.jpcllett.7b00358>

Proton-Transfer-Driven Water Exchange Mechanism in the Na⁺ Solvation Shell

Matti Hellström and Jörg Behler
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Ab Initio Investigation of O–H Dissociation from the Al–OH₂ Complex Using Molecular Dynamics and Neural Network Fitting

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Self-Diffusion of Surface Defects at Copper–Water Interfaces

Suresh Kondati Natarajan and Jörg Behler
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Accurate Neural Network Description of Surface Phonons in Reactive Gas–Surface Dynamics: N₂ + Ru(0001)

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Many-Body Coarse-Grained Interactions Using Gaussian Approximation Potentials

S. T. John and Gábor Csányi
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Data analysis

Antibody Subclass Detection Using Graphene Nanopores

Amir Barati Farimani, Mohammad Heiranian, Kyoungmin Min, and Narayana R. Aluru

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Mesoscale Simulation and Machine Learning of Asphaltene Aggregation Phase Behavior and Molecular Assembly Landscapes

Jiang Wang, Mohit A. Gayatri, and Andrew L. Ferguson

The Journal of Physical Chemistry B **2017** 121 (18), 4923-4944

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Global Sensitivity Analysis with Small Sample Sizes: Ordinary Least Squares Approach

Michael J. Davis, Wei Liu, and Raghu Sivaramakrishnan

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Supervised Machine-Learning-Based Determination of Three-Dimensional Structure of Metallic Nanoparticles

Janis Timoshenko, Deyu Lu, Yuewei Lin, and Anatoly I. Frenkel

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Acceleration of (DFT) model construction

Automated Discovery and Construction of Surface Phase Diagrams Using Machine Learning

Zachary W. Ulissi, Aayush R. Singh, Charlie Tsai, and Jens K. Nørskov

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Improving the Performance of Long-Range-Corrected Exchange-Correlation Functional with an Embedded Neural Network

Qin Liu, JingChun Wang, PengLi Du, LiHong Hu, Xiao Zheng, and GuanHua Chen

The Journal of Physical Chemistry A **2017** 121 (38), 7273-7281

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