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Special Issue Preface

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Physical chemistry stands today at an exciting transition state where the integration of machine learning and data science tools into all corners of the field stands poised to do nothing short of revolutionizing the discipline. These powerful techniques—when appropriately combined with domain knowledge, tools, and expertise—have led to new physical insights, better understanding, accelerated discovery, rational design, and inverse engineering that transcend traditional approaches to materials, molecular, and chemical science and engineering. The primary driver of this trend has been the impressive advances enabled by machine learning, artificial intelligence, and data science tools, ranging from the discovery of novel electronic and optical materials by high-throughput virtual screening, to the massive acceleration of molecular simulations using learned classical force fields with quantum accuracy, to the powering of "self-driving laboratories" for automated chemical discovery. The 2011 White House Materials Genome Initiative (MGI), the 2017 NSF Data-Driven Discovery Science in Chemistry (D3SC) initiative, and the 2019 NSF Big Idea Harnessing the Data Revolution are some of the US federal programs that have provided incentive, attention, momentum, and support to power these advances and help drive the field forward. Necessity is also the mother of invention, and the prevalence of large data sets routinely generated by high-throughput virtual screening or automated experimentation have spurred the need for scalable data science and machine learning techniques to parse, explore, and harness the full power of these voluminous data streams. It bears remembering that physical chemistry is no stranger to machine learning, most visibly in the cheminformatics and quantitative structure property relation (QSPR) work that emerged in the 1980s. Some of the techniques being implemented today are, to some degree, reinventions of these ideas, but others are fundamentally new concepts that have been adopted and adapted from diverse fields including computer vision, manifold learning, and deep learning. This Virtual Special Issue on Machine Learning in Physical Chemistry covering all sections of *The Journal of Physical Chemistry A/B/C* pays tribute to this development, and the relevance and popularity of this topic is reflected in the depth and breadth of excellent articles in this exciting collection.

In *JPC A*, the virtual special issue papers span applications to all aspects of chemical dynamics, molecular property prediction, and electronic structure. The use of machine learning for the efficient determination of accurate ground- and excited-state potential energy surfaces for chemical dynamics and spectroscopy was addressed in the work by Li et al.,[1] Xie et al.,[2] Häkkinen et al.,[3] Houston et al.,[4] Matsuzawa et al.,[5] Priyakumar et al.,[6] Manzhos et al.,[7] Panesi et al.,[8] Ong et al.,[9] Shen and Yarkony,[10] Thompson et al.,[11] Williams and Eisfeld,[12] and Richings and Habershon.[13] Novel machine learning methods were also used for the direct prediction of chemical reaction rates and for the exploration of high-dimensional potential energy surfaces, as in the work of Kästner et al.,[14] Komp and Valleau,[15] Goldsmith and Chen,[16] Meuwly et al.,[17] Wen et al.,[18] and Rinderspacher.[19] A striking array of other chemical properties were also shown to be within the realm of machine learning predictions, including absorption cross sections by Dral et al.,[20] experimental spin states by Kulik et al.,[21] crystal structure prediction by Day et al.,[22] electronic spin couplings from Herrmann et al.,[23] thermochemical properties from Green et al.,[24] site-specific biomolecule reactivity from Swamidass et al.,[25] and dissociation energies by Jiang et al.[26] Machine learning methods were employed for the screening of electronic materials as in the work by Guo et al.,[27] and they were used in combination with spectroscopy methods or the identification of molecules and the characterization thermal distributions, as in the work of Lee et al.,[28] Stoll et al.,[29] and Deshmukh et al.[30] Moreover, a number of papers in the issue addressed the fundamental challenges of electronic structure theory using machine learning methods, including those of Maiti et al.,[31] E et al.,[32] Cui et al.,[33] Curtiss et al.,[34] Crawford et al.,[35] and Vargas-Hernández.[36] And finally, several papers offered perspectives and methodological comparisons on machine learning methods for molecular properties, including those of Gao et al.,[37] Iovanac and Savoie,[38] and Käser, Meuwly et al.[39]

In *JPC B*, the papers address machine learning applications in protein engineering, materials design, free energy and enhanced sampling methods, spectroscopy and microscopy,

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and equations of state and phase diagrams. In ***protein engineering***, Shukla et al.[40] used transfer learning and Markov random fields to predict the functional effects of mutations within homologous protein families, and Petersson et al.[41] employed statistical force fields to learn to classify the effect of thioamide substitutions upon proteolytic activity. Tao et al.[42] analyzed molecular dynamics simulations of an allosteric protein using tree-based models, Markov state models, community analysis, and transition path theory to identify the mechanism of allosteric change. Shea et al.[43] used variational autoencoders to learn a collective variable quantifying amyloid aggregation and produce interpretable latent space embeddings of the assembly process, and Bowers et al.[44] employed classifying autoencoders to expose and correlate the intrinsic properties of amino acid residues to their propensity for amyloid formation. In ***materials design***, Ramprasad et al.[45] trained a multifidelity Gaussian process regression model over high-fidelity experimental data and low-fidelity group contribution predictions to predict the propensity of a polymer to crystallize, and Washburn et al.[46] trained sparse random forest models to predict the glass transition of linear polyurethanes from a small number of informative descriptors. Van Lehn at al.[47] trained convolutional neural networks to efficiently predict hydration free energies of self-assembled monolayers from the time-resolved locations of the interfacial water molecules, and Dumortier and Mossa[48] trained a volumetric convolutional neural network over coarse-grained molecular dynamics simulations to link ionic surfactant network nanostructure with hydration level. Sobh et al.[49] developed a deep learning model to predict and optimize the cure kinetics of thermosetting fiber-reinforced polymer-matrix composites. Angelova et al.[50] performed predictive design of amphiphilic peptide scaffolds using an ensemble of learning algorithms with applications for drug delivery across biological membranes. Nait Amar et al.[51] used gene expression programming to learn an accurate predictive model of A_2XY_6 cubic crystal lattice constants critical to thin film fabrication. Glotzer et al.[52] used spherical harmonics descriptors and unsupervised dimensionality reduction and clustering to identify structural motifs associated with the formation of critical nuclei in supercooled colloidal liquids. Pfaendtner et al.[53] employed variational autoencoders and transfer learning to establish continuous latent embeddings and generative models for data-driven discovery and design of ionic liquids. In an ACS Editors' Choice article, Ferguson et al.[54] combined deep representational learning and Bayesian optimization to perform computational discovery of self-assembling optoelectronic peptides. In ***free energy and enhanced sampling methods***, Tuckerman et al.[55] compared the performance of neural networks, kernel ridge regression, support vector machines, and nearest neighbor methods to learn free energy surfaces from oligopeptide simulation data. Jadrich and Leiding[56] learned a classical reference potential to guide collective ab initio Monte Carlo moves and efficiently generate uncorrelated system configurations within simulations of a noble gas mixture. Shirts et al.[57] applied nonparametric Bayesian time series analysis to long molecular dynamics simulations of solutes in a liquid crystal membrane to resolve transport mechanisms and predict long-time diffusive behaviors. Tiwary et al.[58] learned and optimized reaction coordinates within a basis of order parameters and performed metadynamics to sample the configurational ensemble of flexible protein loops. Dinner et al.[59] developed an extension to the variational approach to conformational dynamics to determine slow collective modes in dynamics systems trajectories by integrating over the lag-time hyperparameter to make the approach more robust and stable. In ***spectroscopy and microscopy***, Buckup et al.[60] used deep learning to extract the states and pathways in relaxation models for excited molecules from time-resolved laser spectroscopy data, and Härkönen et al.[61] employed Bayesian models to analyze, process, and correct coherent anti-Stokes Raman scattering spectra. Liu et al.[62] used image processing and pattern recognition techniques to perform automated prediction of the maturation status of dendritic cells from scanning electron microscopy and atomic force microscopy images. Altman and Grier[63] integrated deep convolutional neural networks with in-line holographic microscopy to efficiently measure the concentration of colloidal dispersions and measure single-particle dynamics. In ***equations of state and phase diagrams***, Zhu and Müller[64] trained artificial neural networks and Gaussian process regression models to learn nonparametric fluid phase equations of state and predict thermophysical fluid properties. Dai and Glotzer[65] employed Gaussian process regression within an active learning framework to minimize the number of samples required to define a materials phase boundary to within a desired precision.

In *JPC C*, the special issue papers describe machine learning and other data science techniques utilized in the scope of nanoparticles and nanostructures; surface and interface processes; electron, ion, and thermal transport; optic, electronic, and optoelectronic materials; and catalysts and catalysis; as well as energy conversion and storage materials and processes. Particular ***target systems*** and compound classes that have been studied in the articles of this issue cover metal−organic and covalent−organic frameworks as well as other porous materials (Desgranges and Delhommelle,[66] Srivastava et al.,[67] Froudakis et al.,[68] Sholl et al.,[69] Krishnapriyan et al.,[70] Walker et al.,[71] Bae et al.,[72] Hasan et al.,[73] Santos et al.[74]); metal and alloy surfaces (Zhang, Jiang et al.,[75] Galvão et al.,[76] del Cueto, Guo et al.,[77] Groenenboom et al.,[78] Rajan et al.,[79] Groenenboom, Anderson et al.,[80] Kroes et al.,[81] Shimizu et al.,[82] Chapman and Ramprasad,[83] Tamblyn et al.[84]); crystalline and amorphous materials (Ni et al.,[85] Wang et al.,[86] Min and Cho,[87] Hu et al.,[88] Shao et al.,[89] Michaelides et al.[90]); nanoclusters and nanoparticles (Kolmogorov et al.,[91] Behler et al.,[92] Daly and Hernandez,[93] Fanourgakis, Froudakis et al.,[94] Baum, Santos, et al.[95]) including defect or doped structures (Barnard et al.,[96] Guan, Liu et al.,[97] Fung, Jiang et al.,[98] Zhou et al.[99]); perovskites (Schrier et al.[100]); organic/polymeric semiconductors (Lu, Lee et al.,[101] Ohuchi et al.[102]) including thin films (Gagliardi et al.,[103] Kimaev and Ricardez-Sandoval[104]) and single molecule junctions (Monti et al.[105]); heterogeneous ternary mixtures (Homma et al.[106]); and liquid crystals (Zavala et al.[107]). The corresponding ***target properties*** and processes that were tackled in the context of these systems cover adsorption; partition functions, isotherms, and other thermodynamic properties; potential energy surfaces and electronic states; optoelectronic and photovoltaic properties; thermal, ionic, and charge conductivity; catalytic activity (e.g., for the hydrogen evolution, oxygen reduction, and CO_2 reduction reactions), reactivity, corrosion, and reactive scattering, including overpotential and work functions; elastic properties; compound formation and optimal product design. A variety of novel and state-of-the-art ***machine learning approaches*** were employed in these studies to elucidate the

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underlying structure−property relationships. A majority of these approaches utilize variations of neural network models (Kolmogorov et al.,[91] Zhang, Jiang et al.,[75] del Cueto, Guo et al.,[77] Behler et al.,[92] Groenenboom, Anderson et al.,[80] Lu, Lee et al.,[101] Zavala et al.,[107] Shin et al.,[108] Hu et al.,[88] Shao et al.,[89] Liu and Kitchin,[109] Kimaev and Ricardez-Sandoval[104] Hasan et al.,[73] Tamblyn et al.[84]), including more advanced versions such as deep, convolutional, adversarial, and recurrent neural network architectures. Other papers leverage active (Min and Cho,[87] Santos et al.[74]) and ensemble learning (Desgranges and Delhommelle[66]) techniques, as well as Bayesian inference models (Yoshizawa et al.,[110] Walker et al.[71]) and unsupervised learning (Monti et al.[105]). Several studies addressed the important issue of adequate featurization (Srivastava et al.,[67] Krishnapriyan et al.,[70] Schrier et al.,[100] Shimizu et al.,[82] Fung, Jiang et al.[98]). Many studies combined data-derived models with more traditional physics-based approaches such as quantum chemistry and molecular dynamics calculations, for data generation (as part of high-throughput screenings), for feature generation, or for the creation of hybrid models.

The new toolbox of techniques and ideas that machine learning and data science have brought to the field makes this a particularly exciting time to be a practitioner in the field of physical chemistry. The excellent collection of thought-provoking articles in this Virtual Special Issue provides a snapshot of this fast-moving field but necessarily represent only a view through the keyhole of the volume of exciting research in this area. We look forward to ever more exciting advances and achievements from our physical chemistry colleagues around the globe.

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Notes

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