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Data Science-Enabled Molecular-to-Systems Engineering for Sustainable Water Technologies

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Abstract

Growing social and economic pressures demand technological innovations that enable the widespread usage of unconventional sources of water (e.g., seawater, grey water). This motivates the emerging fit-for-purpose paradigm, wherein water is provided at the precise quality level of the intended application. Unfortunately, to date, the fundamental advances in materials and nanosystems engineering have been slow to advance this paradigm. We highlight the critical need to bridge scientific research at the molecular and nano-scales and technology development at the device and systems scales for the implementation of sustainable fit-for-purpose water infrastructure. Specifically, we present four pillars from computational and data sciences to bridge between scientific research and technology development, namely *superstructure optimization*, *model-based design of experiments*, *inverse material design*, and *uncertainty quantification*. As such, we highlight opportunities to collaboratively revolutionize water sustainability engineering, but emphasize open communication between data scientists and water-focused researchers using a common vocabulary as a significant hurdle.

Keywords: materials informatics, superstructure optimization, design of experiments, inverse materials design, Bayesian optimization, uncertainty quantification, fit-for-purpose water

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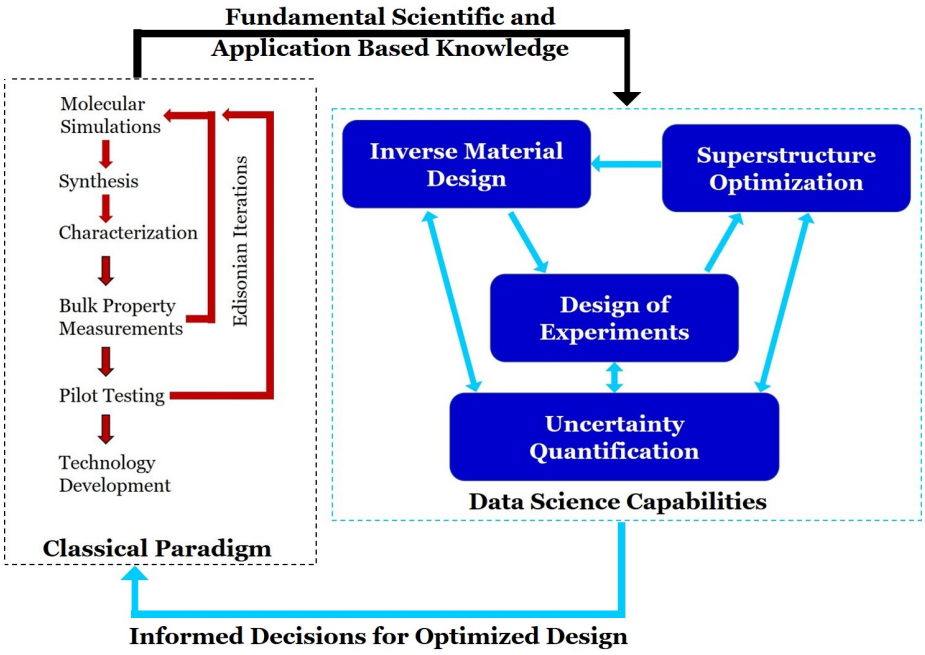

Graphical Abstract

Introduction

Driven by factors such as economic and population growth, aging infrastructure, and increased concerns regarding pollution, water sustainability research is undergoing a paradigm shift to emphasize the highly interconnected and interdependent nature of Earth-water-human systems. Moreover, an increased awareness of the vulnerabilities within existing water supply and management infrastructure has driven interest in the use of non-traditional water resources (e.g., seawater desalination, wastewater reuse) to meet growing demands. As such, several modifications and alternatives to centralized water treatment systems that produce water of a single, potable quality have been proposed. For example, distributed systems that incorporate regenerative treatment technologies tailored to provide fit-for-purpose water closer to its point of use could be

incorporated as part of larger networks [1]. Within this framework, dissolved solutes in waste waters (e.g., nutrients, metal ions) may be viewed as renewable resources that can be recovered. These opportunities have catalyzed research into systems that maximize water reuse and minimize environmental impact by utilizing a series of treatment processes and recycle loops to recover valuable solutes while producing water at a purity level demanded by the requirements of its users. Ultimately, the successful design of these systems will require addressing fundamental questions from the molecular to systems scales related to the development, adoption, and integration of treatment technologies into sustainable networks that ensure robust and resilient infrastructure (Figure 1).

Concurrent with efforts to re-envision the design of the water supply and management infrastructure, advances in chemistry, materials science, and molecular engineering are providing the science and engineering community with unprecedented abilities to design, characterize, and manipulate materials at the molecular through nanoscales [2]. As such, significant opportunities exist to empower the rational design of materials to positively impact water security by coupling this control to the rigorous design of treatment networks through the development of detailed structure-property relationships. For instance, zirconium metal organic frameworks (MOFs) are excellent candidates for the design of selective sorbents that target the removal of harmful organic contaminants from water treated for direct potable reuse [3, 4]. Enabled by thermoresponsive solvents, directional solvent extraction (DSE) [5, 6] can treat high salinity brines from desalination processes using low-cost waste heat as the primary energy input. Due to their ease of operation, modular design, and low energy demands, membrane-based technologies are exciting prospects for clean water technology [7, 8, 9, 10]. Self-assembled block polymer materials allow for the creation of membranes with pore wall chemistries that are readily tailored to enable solute-specific separations and detection. For example, membranes with pore walls tailored to detect and capture metal ions, if appropriately designed, could be used for resource recovery or remediation efforts [11, 12, 13]. Nanocomposite membranes, which are fabricated by incorporating nanomate-

rials into the matrix of conventional membrane structures, can be designed to promote the inactivation of microorganisms that lead to disease and biofouling [14]. Alternatively, nanocomposite membranes can be designed to enable localized solar-thermal heating that enhances membrane distillation processes [15] that may find use in remote and rural regions. While the promise of these materials is exciting, transformative advances for sustainable water have been slow to manifest in practice. Due to their time- and resource-intensive natures, the empirically-driven, heuristic methods that guide most efforts to enhance material properties and device performance are one impediment to realizing this potential. Additionally, these methods are typically applied within the narrow framework of a single process flow and do not incorporate feedback from holistic system design approaches that identify alternative process connectivities or other opportunities for materials deployment.

Accelerating materials discovery necessitates a move away from classical Edisonian methods to principled and data-driven frameworks that can guide material design and process synthesis to overcome the gaps in knowledge that inhibit the translation of new materials and devices from the laboratory scale to effective and sustainable water treatment technologies (Figure 1). In this paper, we present four opportunities for scientists from diverse fields to work at the intersections of materials science, computational science, civil and environmental engineering, mechanical engineering, and chemical engineering to revolutionize water sustainability engineering by fully realizing the *fourth paradigm* of materials science [16] (Figure 2).

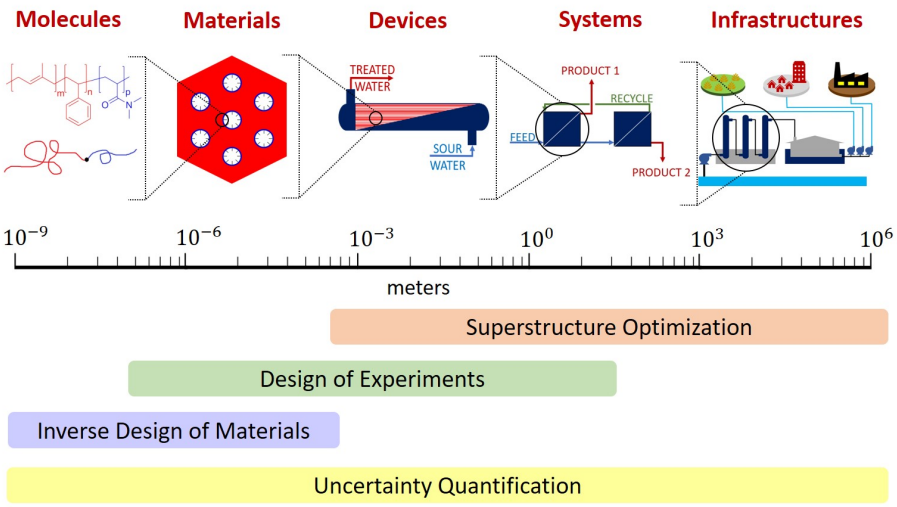

Figure 1: In the bottom-up approach to sustainable water engineering, new (macro)molecular structures enable novel materials with desired properties that are incorporated into devices for target applications. These devices are then integrated into process networks wherein the system topology enables non-traditional applications such as nutrient recovery and wastewater treatment which form an essential part of the water distribution infrastructure in the fit-for-use paradigm. Computational and data science tools can accelerate this process to facilitate top-down analysis and discovery of materials. In the top-down approach, superstructure optimization is used to design resilient infrastructures and novel system configuration for specific water purification and solute recovery applications. These designs dictate targets for material properties that guide the inverse design of materials. Likewise, bottom-up analysis facilitates rapid screening of new materials in the context of fully optimized systems and infrastructure. Multiscale uncertainty quantification and propagation unite all the computational and data science tools into a holistic molecules-to-infrastructures framework.

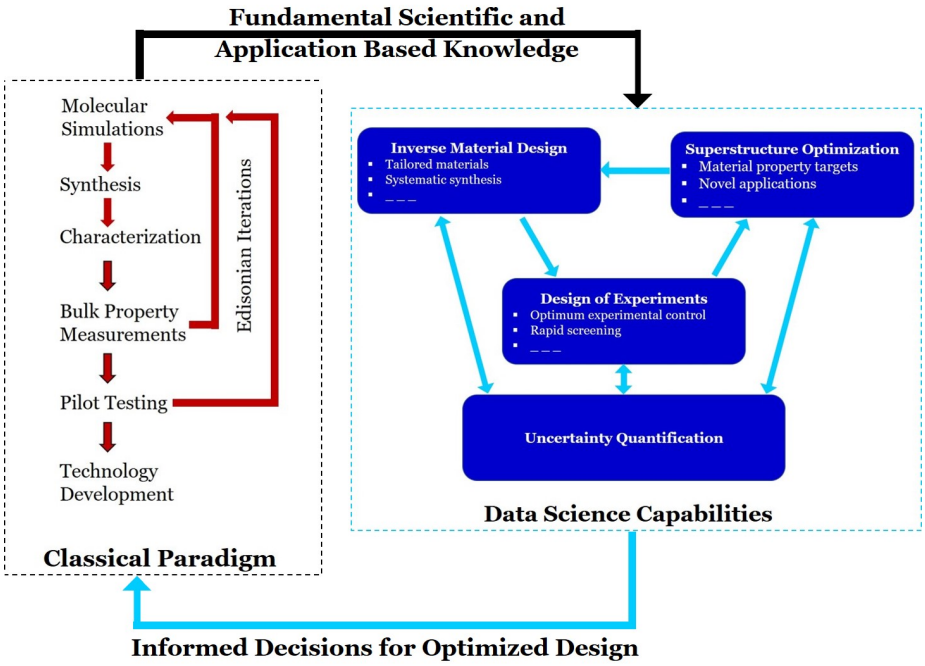

Figure 2: In the proposed paradigm, data science capabilities optimize the materials discovery process by maximizing the amount of useful information gained from each iteration and enabling multiscale analysis.

Opportunity 1: Superstructure optimization enables rapid bottom-up and top-down analysis

Superstructure optimization is a classical paradigm in process systems engineering with ubiquitous applications including water distribution networks [17, 18], water supply chains [19], and sensor placement [20]. First, the modeler postulates a superstructure at the desired length scale that encodes all possible system configurations. Next, an optimization problem is formulated over the superstructure. For example, minimize water production cost by searching over all feasible combinations of design choices (e.g., selection and size of equipment, flow rates). Finally, the optimization problem is solved numerically, resulting in one (or more) designs with optimal topology (integer decisions) and operating conditions (continuous decisions) identified. Often, superstructure optimization elucidates novel system topologies. For example, Du *et al.* [21] discovered permeate split designs for a single-feed, multi-product seawater reverse osmosis desalination network using superstructure optimization. Thus, demonstrating how commercially-available materials, if optimally integrated into devices and systems, can overcome operational challenges such as boron removal. Yenkie *et al.* use superstructure optimization to calculate quantitative performance thresholds that define when various separation pathways minimize production costs in an integrated biorefinery [22]. We foresee superstructure optimization playing a pivotal role in establishing holistic molecules-to-systems design frameworks that encompass all aspects of sustainable water.

Extending established top-down superstructure optimization methods to encompass emerging fit-for-purpose paradigms and the additional constraints needed to address resource recovery and water reuse can help to focus research efforts into these highly-integrated, complex systems on the most impactful areas of water sustainability research. In this domain, there is a great need to understand the basic cost and performance drivers [23] for new sustainable water technologies in the context of existing or future infrastructure, regulations, and public opinion with many stakeholders [24]. Emerging efforts in this arena

are focused on establishing top-down guidance at the device level by establishing the materials property targets needed to enable novel process configurations [21, 25] (Figure 3a). Moreover, top-down approaches are beginning to span the divide between the materials and systems scale by embedding empirical correlations that guide materials selection within the optimization framework. For example, the Robeson plot, which quantifies the trade-off between permeability and selectivity for membranes was considered when optimizing the design of binary gas separation systems [26, 27, 28]. Incorporating these structure-property relationships into the optimization framework can both quantify the relative importance of competing material properties (Figure 3b) and elucidate the potential for performance gains at the systems level from technological breakthroughs, i.e., shifting the Robeson plot. As such, superstructure optimization frameworks of the future could inform both *how* to design and manufacture nanostructured materials and how to integrate them into resilient infrastructures with many competing objectives.

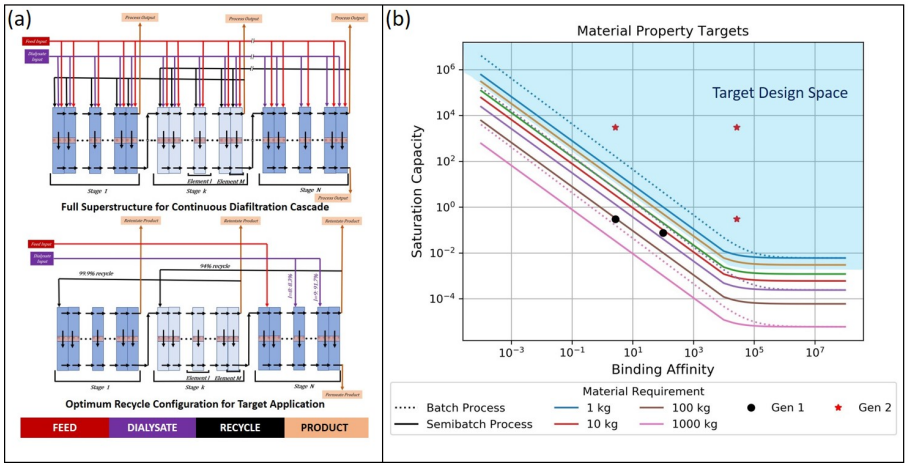

Figure 3: **(a) Superstructure Optimization:** In [25] we propose a superstructure optimization strategy to intensify membrane separations using continuous diafiltration cascades. The full superstructure formulation encoding multiple recycle strategies for the cascade is shown at the top. A solution showing optimum strategies for feed injection, product withdawal and recycle is obtained by eliminating streams whose flow rate is zero and is shown in the bottom of the figure. The optimum configuration is obtained after a sensitivity analysis to identify membrane selectivity values needed to outperform existing technologies for lithium ion battery recycling. **(b) Material Property Targets:** In another work, we studied the removal of heavy metal contaminants from water using adsorptive nanoprous membranes. Targets for competing material properties are defined by operational (process) and consumer needs. Generation 1 materials (baseline) already exist. Generation 2 materials are tailored for target applications such as heavy metal removal, and can be designed by significantly improving any one of the two competing material properties (vertical or horizontal movement into the target design space), or by modest improvements in both material properties (diagonal movement into target design space)

Superstructure optimization is also well-positioned to guide molecular engineering via bottom-up analysis. For already characterized materials, rigorous superstructure optimization enables rapid comparison against competing technologies in the context of fully optimized systems and can identify potential applications for materials. Large databases of material properties, derived from high throughput experiments and/or computations, now enable data-driven discovery via machine learning and data science methods which has given rise to materials informatics, the so-called *fourth paradigm* of materials science [16]. Recent efforts propose superstructure optimization formulations to design crystalline material structures, such as MOFs, based on the constraints imposed by process separations.[29, 30] Extending this bottom-up analysis to soft materials, such as polymeric membranes, remains a challenge. Although empirical structure-property relationships exist for some polymer structures [13], the fundamental understanding of the molecular interactions and transport mechanisms that solute-specific separations are still rudimentary [31]. Nevertheless, we anticipate materials informatics will lead to new insights and more accurate structure-property relationships needed for direct molecules-to-systems optimization. Furthermore, we foresee opportunities to combine molecular simulations and superstructure optimization to enable high-throughout screening of emerging materials using systems-scale metrics (e.g., separation selectivity, energy usage, product cost) as benchmarks for performance.

Opportunity 2: Model based design of experiments accelerates hypothesis driven discovery

A fundamental challenge in the hypothesis driven discovery currently utilized to establish structure-property relationships is designing experimental campaigns that maximize useful information gained [32]. Classical design of experiments techniques (e.g., multi-level factorial, partial factorial designs) help establish empirical models (e.g., polynomial response surfaces), which although predictive, rarely offer insights into fundamental scientific phenomena. In con-

trast, model based design of experiments (MBDOE) frameworks directly consider differential and/or algebraic equations grounded in scientific and engineering fundamentals (e.g., conservation laws, thermodynamics) in their formulation. MBDOE techniques are popular in biology, pharmacology, and reaction engineering, as these experiments are often time- and resource-intensive. For example, Laínez-Aguirre *et al.* use a fully Bayesian MBDOE framework to estimate nonlinear differential algebraic pharmacokinetics models which enable dosing regimens optimized to individual patients [33]. In another recent example, Lu et al. [34] use MBDOE to discern between competing kinetics models for chemical-looping combustion. Despite the fact that similar challenges exist in sustainable water treatment (e.g., scheduling of membrane cleaning, identifying degradation pathways of contaminants), MBDOE techniques have seldom been leveraged in this arena.

We foresee MBDOE as an essential paradigm to ensure that the most useful data is collected when establishing structure-property relationships. As mentioned in Opportunity 1, the transport, thermodynamics, and reaction mechanisms that enable water treatment technologies are often not sufficiently understood. We believe it is possible to postulate model collections where each model corresponds to specific scientific hypotheses about the dominant physical and chemical phenomena. MBDOE then facilitates design of multifaceted experimental campaigns to discern the most probable subset of models (hypotheses). This proposed paradigm is especially powerful in the elucidation of regimes where a single mechanism dominates and the identification of conditions where transitions between mechanisms occur. For example, it could potentially be utilized to elucidate where transport through membranes transitions from being governed by a solution-diffusion mechanism to a pore flow dominated regime. Moreover, MBDOE can enable the design and analysis of high throughput transient experiments, thereby eliminating the time required for a test system to reach equilibrium.[35] This capability may be particularly useful when testing new technologies against realistic feed solutions. Often materials characterization is executed using idealized solutions that contain a single dissolved com-

ponent. In practice, however, water treatment technologies are challenged by complex, multi-component solutions whose composition varies with time. As such, there is a critical need to assess material and device performance in a broader spectrum of feed solution conditions. In this regard, the proposed capabilities of MBDOE would greatly accelerate development of sustainable water technologies that can robustly operate over wide operating ranges with many contaminants.

Opportunity 3: Adaptive design of experiments enables systematic inverse material design

The convergence of materials informatics and data science with physical and synthetic chemistry to establish inverse material design methods is imminent. The goal is to predict computationally (macro)molecular and/or self-assembled structures that archive target material properties. The nearly limitless design space of candidate materials cannot be enumerated with conventional high throughput computational screening methods [36, 37]. Instead, in the adaptive design of experiments paradigm, a surrogate or machine learning model is constructed to predict material properties (e.g., solubility, tensile strength) from input design variables (e.g., molecular structure, alloy composition). Design of experiments methods then postulate new materials to synthesize or simulate using the surrogate model. Recent successful applications include nanofabrication and nanoparticle self-assembly [38, 39], drug design [40], and high strength alloys [41]. In Bayesian optimization methods, domain specific knowledge and observed data are incorporated into the prior distribution of the Gaussian Process (GP) surrogate model.[42] The computationally inexpensive GP model enables optimization of experimental conditions that balance *exploration* (sampling regions of high uncertainty) and *exploitation* (sampling regions with best predicted material performance). New observations are leveraged to improve the GP surrogate model using Bayes rule, making the procedure adaptive (self-learning). Adaptive designs have been shown to outperform pure exploitation approaches

in several studies [41].

Data-driven inverse materials design methods will soon enable novel sustainable water technologies. Yet these applications pose numerous challenges and opportunities. Thus far, many adaptive design of experiments successes are with either limited design spaces (e.g., ternary alloys) or crystalline materials with well-defined and predictable structures. In contrast, soft materials such as polymeric and nanocomposite membranes have extremely large design spaces because they are processed far from equilibrium and therefore, possess non-equilibrium structures. New mathematical descriptions grounded in physical and chemical understanding are needed to encode all of the design choices for soft materials. Depending on the target material properties, inexpensive high throughput computational predictions may not be available. In such cases, molecular simulations are often needed to elucidate the self assembly process and ultimately predict structure and properties of soft materials [43]. This trade-off between computational expense and molecular-scale detail underscores the need for systematic methods to guide inverse materials design. Finally, water treatment technologies are often multifaceted and utilize a combination of phenomena to achieve their goal. This broad design space necessities advances in multiobjective and multifidelity adaptive design of experiments methods that can both navigate competing design goals (material targets) and assimilate heterogenous data from many sources.

Opportunity 4: Multiscale uncertainty quantification derisks technology development

Ultimately, using data-science to help bridge the gap between materials and water sustainability engineering has the promise to inform the molecular-scale design of devices and systems that enable the development of resilient, secure, and sustainable infrastructure. We believe optimization under uncertainty, a well-established technique for risk mitigation in supply chains and water recycle networks [44], will play a critical role in realizing the fit-for-purpose water

paradigm, with data science methods informing uncertainty sets (probability distributions) [45, 46] as information is propagated over the relevant design scales. Recently, Bhat *et al.* demonstrated how Bayesian uncertainty upscaling, which encompasses modeling fundamental thermodynamic and transport phenomena, bench-scale demonstrations, and superstructure optimization under uncertainty, can derisk CO_2 capture technologies. [47] As illustrated in Figure 2, we see great needs and opportunities to expand formula uncertainty quantification across molecular, material, device, systems, and infrastructure scales for suistainable water. For example, Edisonian iterations between molecular simulations and experiments are at the core of the existing materials discovery paradigm (Figure 2). Yet emerging UQ frameworks enable rigorous calibration of force field parameters and assessment of predictions from molecular simulations [48]. We see opportunities to develop new multi-fidelity design of experiments algorithms to co-optimize allocation of computational and physical resources in order to establish systematic feedback loops between molecular simulations and physical experiments. Supported by rigorous statistical analysis, molecular simulations and physical experiments provide rich heterogeneous datasets with uncertainty estimates to derive (differential) algebraic surrogate (i.e., reduced order, timescale bridging) models that enable computationally tractable optimization under uncertainty [49, 50]. Here, there are significant opportunities to extend the surrogate modeling paradigm to grey-box models, which combine physics-informed equations with a data-driven component that quantifies model form uncertainty [47, 51]. Using these uncertainties, superstructure optimization can provide quantitative material property and cost targets that serve as input for inverse materials design. Critically, this vision necessitates integrating innovations in data science and UQ with fundamental scientific and engineering principles to accelerate sustainable water technologies faster than both fields working separately.

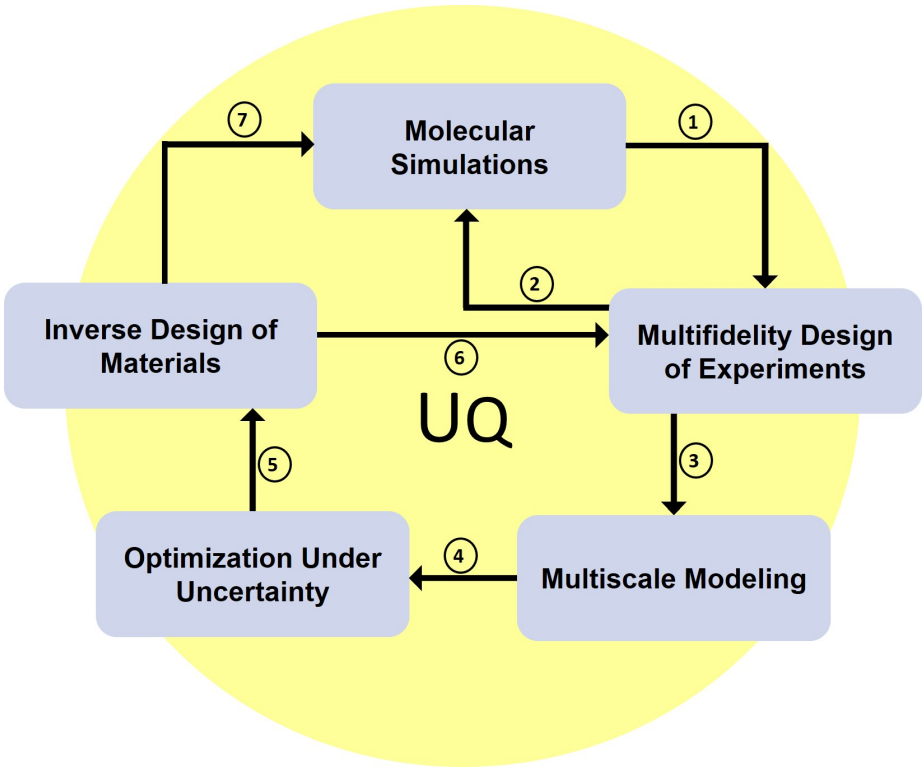

Figure 4: Uncertainty quantification (UQ) unifies all aspects of sustainable water engineering into comprehensive molecular-to-infrastructure design framework. Together, molecular simulations and UQ enables accurate force-field selection and calibration. This provides molecular structure and material property predictions with quantified uncertainties ① to inform laboratory experiments and DOE. Likewise, multifaceted laboratory experiments provide data ② for molecular simulation validation, creating a feedback loop. Multifideltiy design of both laboratory and computational experiments provides rich heterogeneous data with uncertainty estimations ③ for multiscale model reduction. This then provides tractable surrogate (low fidelity) models with quantified uncertainty descriptions ④, which are inputs for superstructure optimization under uncertainty. These optimization problems elucidate possible applications for new materials, material property targets, and device, system and infrastructure designs that are robust to uncertainties (variable feed compositions, rare event, etc.). These results, especially property targets, ⑤ are inputs for inverse design of materials. Adaptive design of experiments (e.g., Bayesian optimization) then proposes tailored materials, ⑥ and ⑦, for synthesis, laboratory characterization, and computational exploration.

Conclusions

In this paper, we highlight four opportunities for emerging data-science frameworks to establish new paradigms for sustainable water technologies: superstructure optimization, design of experiments, inverse material design and uncertainty quantification. Many engineering challenges in the sustainable water domain are likely intractable for existing computational paradigms, but provide timely and impactful applications to motivate methodological advances in data and computer science. Data-driven tools cannot alone revolutionize the field. Instead, we foresee collaborative efforts that combine domain specific knowledge with machine learning paradigms as essential to realizing holistic molecules-to-infrastructures engineering frameworks that can usher in the next era of materials discovery for sustainable water enterprises.

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Conflict of interest statement

Nothing to declare.

References and recommended reading

[1] K. R. Zodrow, Q. Li, R. M. Buono, W. Chen, G. Daigger, L. Dueñas-Osorio, M. Elimelech, X. Huang, G. Jiang, J. H. Kim, B. E. Logan, D. L. Sedlak, P. Westerhoff, P. J. Alvarez, Advanced Materials, Technologies, and Complex Systems Analyses: Emerging Opportunities to Enhance Urban Water Security, Environmental Science and Technology 51 (18) (2017) 10274–10281,

· This paper addresses the innovations needed in urban water systems due to the strain on freshwater sources caused by increasing population, pollution, aging infrastructure and climate change. It advocates the integration of advanced materials as well as complex system analysis and modeling for the development of a sustainable and resilient urban water supply system. doi:10.1021/acs.est.7b01679.

[2] P. J. J. Alvarez, C. K. Chan, M. Elimelech, N. J. Halas, D. Villagrán, Emerging opportunities for nanotechnology to enhance water security, Nature Nanotechnology 13 (2018) 634–641. doi:10.1038/s41565-018-0203-2.

[3] B. Van de Voorde, B. Bueken, J. Denayer, D. De Vos, Adsorptive separation on metal-organic frameworks in the liquid phase., Chemical Society Reviews 43 (16) (2014) 5766–88. doi:10.1039/c4cs00006d.

[4] R. J. Drout, L. Robison, Z. Chen, T. Islamoglu, O. K. Farha, Zirconium Metal Organic Frameworks for Organic Pollutant Adsorption, Trends in Chemistry 1 (3) (2019) 304–317. doi:10.1016/j.trechm.2019.03.010.

[5] A. Bajpayee, T. Luo, A. Muto, G. Chen, Very low temperature membrane-free desalination by directional solvent extraction, Energy and Environmental Science 4 (5) (2011) 1672–1675. doi:10.1039/c1ee01027a.

[6] C. Boo, R. K. Winton, K. M. Conway, N. Y. Yip, Membrane-less and Non-Evaporative Desalination of Hypersaline Brines by Temperature Swing Solvent Extraction, Environmental Science & Technology Letters (2019) 1–6doi:10.1021/acs.estlett.9b00182.

[7] M. Elimelech, W. A. Phillip, The future of seawater desalination: Energy, technology, and the environment, Science 333 (6043) (2011) 712–717. doi:10.1126/science.1200488.

[8] J. R. Werber, C. O. Osuji, M. Elimelech, Materials for next-generation

desalination and water purification membranes, Nature Reviews Materials 1 (16018) (2016) 1–16. doi:10.1038/natrevmats.2016.18.

[9] A. G. Fane, R. Wang, M. X. Hu, Synthetic membranes for water purification: Status and future, Angewandte Chemie - International Edition 54 (11) (2015) 3368–3386. doi:10.1002/anie.201409783.

[10] A. Lee, J. W. Elam, S. B. Darling, Membrane materials for water purification: Design, development, and application, Environmental Science: Water Research and Technology 2 (1) (2016) 17–42. doi:10.1039/c5ew00159e.

[11] Y. Zhang, J. R. Vallin, J. K. Sahoo, F. Gao, B. W. Boudouris, J. Matthew, W. A. Phillip, Y. Zhang, J. R. Vallin, J. K. Sahoo, F. Gao, P. M. J. Webber, P. W. A. Phillip, M. Hall, High-Affinity Detection and Capture of Heavy Metal Ions using Block Polymer Composite Membranes, ACS Central Science 4 (12) (2018) 1697–1707.

[12] J. L. Weidman, R. A. Mulvenna, B. W. Boudouris, W. A. Phillip, Nanoporous Block Polymer Thin Films Functionalized with Bio-Inspired Ligands for the Efficient Capture of Heavy Metal Ions from Water, ACS Applied Materials and Interfaces 9 (22) (2017) 19152–19160. arXiv:arXiv:1408.1149, doi:10.1021/acsami.7b04603.

[13] Y. Zhang, N. E. Almodovar-Arbelo, J. L. Weidman, D. S. Corti, B. W. Boudouris, W. A. Phillip, Fit-for-purpose block polymer membranes molecularly engineered for water treatment, npj Clean Water 1 (2) (2018) 1–14, · This paper discusses the potential of nanporous membranes derived from block polymers precursors to advance water treatment technologies in the arenas of desalination and hybrid water purification and resource recovery processes. It provides a comprehensive review of the experimental and computational efforts undertaken for the development of membranes for the advanced water treatment systems and an insight into the hurdles that must be overcome for their widespread technological implementation. doi:10.1038/s41545-018-0002-1.

[14] X. Lu, X. Feng, J. R. Werber, C. Chu, I. Zucker, J.-H. Kim, C. O. Osuji, M. Elimelech, Enhanced antibacterial activity through the controlled alignment of graphene oxide nanosheets, Proceedings of the National Academy of Sciences 114 (46) (2017) E9793–E9801. doi:10.1073/pnas.1710996114.

[15] P. D. Dongare, A. Alabastri, S. Pedersen, K. R. Zodrow, Nanophotonics-enabled solar membrane distillation for off-grid water purification, Proceedings of the National Academy of Sciences 114 (27) (2017) 6936–6941. doi:10.1073/pnas.1701835114.

[16] A. Agrawal, A. Choudhary, Perspective: Materials informatics and big data: Realization of the "fourth paradigm" of science in materials science, APL Materials 4 (053208) (2016) 1–11. doi:10.1063/1.4946894.

[17] E. Buabeng-baidoo, T. Majozi, Effective Synthesis and Optimization Framework for Integrated Water and Membrane Networks : A Focus on Reverse Osmosis Membranes, Industrial and Engineering Chemistry Research 54 (38) (2015) 9394–9406. doi:10.1021/acs.iecr.5b01803.

[18] E. Ahmetović, N. Ibrić, Z. Kravanja, I. E. Grossmann, Water and energy integration: A comprehensive literature review of non-isothermal water network synthesis, Computers and Chemical Engineering 82 (2015) 144–171. doi:10.1016/j.compchemeng.2015.06.011.

[19] Y. Chen, L. He, J. Li, S. Zhang, Multi-criteria design of shale-gas-water supply chains and production systems towards optimal life cycle economics and greenhouse gas emissions under uncertainty, Computers and Chemical Engineering 109 (2018) 216–235. doi:https://doi.org/10.1016/j.compchemeng.2017.11.014.

[20] R. Mukherjee, U. M. Diwekar, A. Vaseasht, Optimal sensor placement with mitigation strategy for water network systems under uncertainty, Computers and Chemical Engineering 103 (2017) 91 – 102. doi:10.1016/j.compchemeng.2017.03.014.

[21] Y. Du, Y. Liu, S. Zhang, Y. Xu, Optimization of seawater reverse osmosis desalination networks with permeate split design considering boron removal, Industrial and Engineering Chemistry Research 55 (50) (2016) 12860 – 12879,

· This article studies seawater reverse osmosis using a rigorous model considering a solution-diffusion mechanism of transport across the membrane, as well as membrane fouling criteria. The analysis for a single feed, multi-product network suggests novel permeate split designs, identifies the best suited membrane materials that reduced cost and energy consumption by operating smaller equipment in addition to identify non-constant optimum annual operating conditions over four years of operation. doi:10.1021/acs.iecr.6b02225.

[22] K. M. Yenkie, W. Wu, C. T. Maravelias, Biotechnology for Biofuels Synthesis and analysis of separation networks for the recovery of intracellular chemicals generated from microbial based conversions, Biotechnology for Biofuels 10 (1) (2017) 1–22. doi:10.1186/s13068-017-0804-2.

[23] T. V. Bartholomew, N. S. Siefert, M. S. Mauter, Cost Optimization of Osmotically Assisted Reverse Osmosis, Environmental Science and Technology 52 (20) (2018) 11813–11821. doi:10.1021/acs.est.8b02771.

[24] A. W. Dowling, G. Ruiz-Mercado, V. M. Zavala, A framework for multi-stakeholder decision-making and conflict resolution, Computers and Chemical Engineering 90 (2016) 136 – 150. doi:10.1016/j.compchemeng.2016.03.034.

[25] E. A. Eugene, W. A. Phillip, A. W. Dowling, Material Property Goals to Enable Continuous Diafiltration Cascades for Lithium-Ion Battery Recycling, Proceedings for Foundations of Computer Aided Process Design (FOCAPD 2019) Accepted.

[26] R. Zarca, A. Ortiz, D. Gorri, L. T. Biegler, I. Ortiz, Optimized distillation coupled with state-of-the-art membranes for propylene purification, Journal

of Membrane Science 556 (2018) 321–328. doi:10.1016/j.memsci.2018.04.016.

[27] B. Ohs, J. Lohaus, M. Wessling, Optimization of membrane based nitrogen removal from natural gas, Journal of Membrane Science 498 (2016) 291–301. doi:10.1016/j.memsci.2015.10.007.

[28] M. Scholz, M. Alders, T. Lohaus, M. Wessling, Structural optimization of membrane-based biogas upgrading processes, Journal of Membrane Science 474 (2015) 1–10. doi:10.1016/j.memsci.2014.08.032.

[29] C. L. Hanselman, C. E. Gounaris, A mathematical optimization framework for the design of nanopatterned surfaces, AIChE Journal 62 (9) (2016) 3250–3263. doi:10.1002/aic.15359.

[30] E. L. First, C. E. Gounaris, C. A. Floudas, Predictive Framework for Shape-Selective Separations in Three- Dimensional Zeolites and Metal Organic Frameworks, Langmuir 29 (18) (2013) 5599 – 5608. doi:10.1021/la400547a.

[31] H. B. Park, J. Kamcev, L. M. Robeson, M. Elimelech, B. D. Freeman, Maximizing the right stuff: The trade-off between membrane permeability and selectivity, Science 356 (6343) (2017) 1–10. doi:10.1126/science.aab0530.

[32] G. Franceschini, S. Macchietto, Model-based design of experiments for parameter precision: State of the art, Chemical Engineering Science 63 (19) (2008) 4846–4872. doi:10.1016/j.ces.2007.11.034.

[33] J. M. Laínez-Aguirre, L. Mockus, G. V. Reklaitis, A stochastic programming approach for the Bayesian experimental design of nonlinear systems, Computers and Chemical Engineering 72 (2015) 312–324,
· This paper formulates a fully Bayesian design of experiments problem for a pharmacokinetics study. The study solves the problem using stochastic programming (optimization over a probability distribution) to capture the

inherent uncertainties in the process. The study finds up to 86% reduction in the number of experiments needed to characterize the pharmacokinetics of the drugs studied. doi:10.1016/j.compchemeng.2014.06.006.

[34] L. Han, Z. Zhou, G. M. Bollas, Model-based analysis of chemical-looping combustion experiments. Part II: Optimal design of CH_4-NiO reduction experiments, AIChE Journal 62 (7) (2016) 2432–2446. doi:10.1002/aic.15242.

[35] F. Galvanin, E. Cao, N. Al-Rifai, A. Gavriilidis, V. Dua, A joint model-based experimental design approach for the identification of kinetic models in continuous flow laboratory reactors, Computers and Chemical Engineering 95 (2016) 202 – 215. doi:10.1016/j.compchemeng.2016.05.009.

[36] E. A. Pfeif, K. Kroenlein, Perspective: Data infrastructure for high throughput materials discovery, APL Materials 4 (5) (2016) 1–12. doi:10.1063/1.4942634.

[37] T. Lookman, P. V. Balachandran, D. Xue, J. Hogden, J. Theiler, Statistical inference and adaptive design for materials discovery, Current Opinion in Solid State and Materials Science 21 (3) (2017) 121 – 128. doi:10.1016/j.cossms.2016.10.002.

[38] M. J. Casciato, S. Kim, J. C. Lu, D. W. Hess, M. A. Grover, Optimization of a carbon dioxide-assisted nanoparticle deposition process using sequential experimental design with adaptive design space, Industrial and Engineering Chemistry Research 51 (11) (2012) 4363–4370,
· This study introduce an adaptive design technique called Layer of Experiments with Adaptive Combined Design (LoE/ACD), a novel experimental design methodology for both model discrimination and parameter estimation. The methodology considerably reduced the design space for a carbon dioxide nanoparticle deposition process under significant uncertainty in addition to an engineering tolerance requirement. doi:10.1021/ie2028574.

[39] H. Kim, J. T. Vastola, S. Kim, J. C. Lu, M. A. Grover, Batch sequential minimum energy design with design-region adaptation, Journal of Quality Technology 49 (1) (2017) 11–26. doi:10.1080/00224065.2017.11918182.

[40] R. Gómez-Bombarelli, J. N. Wei, D. Duvenaud, J. M. Hernández-Lobato, B. Sánchez-Lengeling, D. Sheberla, J. Aguilera-Iparraguirre, T. D. Hirzel, R. P. Adams, A. Aspuru-Guzik, Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules, ACS Central Science 4 (2) (2018) 268–276,

· This study demonstrates an adaptive design technique for the discovery of drug-like molecules. The novelty of the approach allows the representation of discrete molecules in a continuous multidimensional space that enables efficienct gradient-based optimization and Bayesian inference to find new molecular structures. doi:10.1021/acscentsci.7b00572.

[41] D. Xue, P. V. Balachandran, J. Hogden, J. Theiler, D. Xue, T. Lookman, Accelerated search for materials with targeted properties by adaptive design, Nature Communications 7 (11241) (2016) 1–9. doi:10.1038/ncomms11241.

[42] P. I. Frazier, J. Wang, Bayesian Optimization for Materials Design, Springer International Publishing, Cham, 2016, pp. 45–75. doi:10.1007/978-3-319-23871-5_3.

[43] V. S. Rathee, S. Qu, W. A. Phillip, J. K. Whitmer, A coarse-grained thermodynamic model for the predictive engineering of valence-selective membranes, Molecular Systems Design and Engineering 1 (3) (2016) 301–312. doi:10.1039/C6ME00045B.

[44] I. E. Grossmann, R. M. Apap, B. A. Calfa, P. García-herreros, Q. Zhang, Recent advances in mathematical programming techniques for the optimization of process systems under uncertainty, Computers and Chemical Engineering 91 (2016) 3–14. doi:10.1016/j.compchemeng.2016.03.002.

[45] C. Ning, F. You, Data-driven stochastic robust optimization: General computational framework and algorithm leveraging machine learning for optimization under uncertainty in the big data era, Computers and Chemical Engineering 111 (2018) 115–133. doi:10.1016/j.compchemeng.2017.12.015.

[46] B. A. Calfa, I. E. Grossmann, A. Agarwal, S. J. Bury, J. M. Wassick, Data-driven individual and joint chance-constrained optimization via kernel smoothing, Computers and Chemical Engineering 78 (2015) 51–69. doi:10.1016/j.compchemeng.2015.04.012.

[47] K. S. Bhat, D. S. Mebane, P. Mahapatra, C. B. Storlie, Upscaling uncertainty with dynamic discrepancy for a multi-scale carbon capture system, Journal of the American Statistical Association 112 (520) (2017) 1453–1467,

· This study of carbon dioxide capture systems extends the Kennedy O'Hagan methodology to study the inadequacies of dynamic models, specifically the reaction-diffusion kinetic model. They further demonstrate the significance of propagating the uncertainty via the Bayesian upscaling process.

. doi:10.1080/01621459.2017.1295863.

[48] S. T. Reeve, A. Strachan, Error correction in multi-fidelity molecular dynamics simulations using functional uncertainty quantification, Journal of Computational Physics 334 (2017) 207–220. doi:10.1016/j.jcp.2016.12.039.

[49] A. Cozad, N. V. Sahinidis, D. C. Miller, A combined first-principles and data-driven approach to model building, Computers and Chemical Engineering 73 (2015) 116–127. doi:10.1016/j.compchemeng.2014.11.010.

[50] L. T. Biegler, Y. dong Lang, W. Lin, Multi-scale optimization for process systems engineering, Computers and Chemical Engineering 60 (2014) 17–30. doi:10.1016/j.compchemeng.2013.07.009.

[51] K. Li, P. Mahapatra, K. S. , D. C. Miller, D. S. Mebane, D. C. McHugh, J.-F. Dietiker, T. Li, J. Spenik, A. Kiviste, X. Sun, S. Sundaresan, E. Ryan, D. Engel, C. Dale, Multi-scale modeling of an amine sorbent fluidized bed adsorber with dynamic discrepancy reduced modeling, Reaction Chemistry and Engineering 2 (2017) 550–560. doi:10.1039/C7RE00040E.