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Integrating computational chemistry with environmental policy: A systems approach to contaminant mitigation in U.S. Drinking Water Systems

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Abstract

Emerging contaminants such as PFAS, PPCPs, EDCs, and heavy metals present complex challenges to U.S. drinking water systems, often evading conventional treatment and regulatory oversight. These in silico methods offer predictive capabilities for contaminant fate, toxicity, and transport, enabling high-throughput screening and mechanistic insight at molecular scales. Despite their scientific maturity, regulatory uptake remains limited due to lack of standardization, temporal misalignment with policy cycles, and poor scale translation to field-level applications. Approximately 41% of reviewed studies demonstrated policy relevance, interfacing with EPA programs such as ToxCast, UCMR, and TSCA. Systems thinking approaches, including Life-Cycle Assessment (LCA) and Integrated Assessment Models (IAMs), show promise in bridging molecular data with decision-making tools. The review advocates for transdisciplinary frameworks that align computational innovation with adaptive governance, emphasizing co-development, transparency, and regulatory receptivity. Advancing such integration is critical to modernizing environmental risk assessment and safeguarding public health amid increasing chemical complexity and infrastructure vulnerability.

Keywords: Polyfluoroalkyl Substances; Endocrine-Disrupting Compounds; QSAR Modeling; DFT Modeling; Systems-Based Risk Assessment

1. Introduction

Ensuring the safety and quality of drinking water remains a pressing public health concern in the United States. Despite regulatory advances under the Safe Drinking Water Act (SDWA) and the establishment of maximum contaminant levels (MCLs) for over 90 substances, an increasing number of emerging contaminants (ECs) pose significant challenges to conventional water treatment and risk assessment protocols [1].

Among the most scrutinized ECs are per- and polyfluoroalkyl substances (PFAS), pharmaceuticals and personal care products (PPCPs), disinfection by-products (DBPs), endocrine-disrupting compounds (EDCs), and heavy metals such as lead, arsenic, and hexavalent chromium. PFAS, often referred to as “forever chemicals” due to their environmental persistence, have been linked to immunotoxicity, developmental issues, and carcinogenicity, yet they remain largely unregulated in many states [2]. Similarly, PPCPs and EDCs, originating from human waste streams and agricultural runoff, are frequently detected in surface water at trace levels that evade traditional treatment yet may exert sub-lethal and cumulative effects on human health [3, 4]

Disinfection by-products, such as trihalomethanes (THMs) and haloacetic acids (HAAs), are formed as unintended consequences of chlorination, posing mutagenic and carcinogenic risks [3, 4]. Lead contamination, made infamous by the Flint water crisis, continues to represent a major equity issue, particularly in marginalized communities with aging

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infrastructure. These contaminants often co-occur, interact synergistically or antagonistically, and exhibit non-linear dose-response relationships, which complicates exposure modeling and regulatory thresholds [5].

Despite the presence of national monitoring frameworks like the Unregulated Contaminant Monitoring Rule (UCMR) and Toxic Substances Control Act (TSCA), the gap between environmental science and policymaking has resulted in reactive rather than proactive governance [6]. In this context, there is a critical need for innovative tools and transdisciplinary approaches that can elucidate contaminant behavior at the molecular level, forecast environmental persistence, and support data-driven mitigation policies.

1.1. Computational Chemistry in Environmental Science

Computational chemistry has emerged as a vital component of environmental science, offering predictive capabilities that surpass the spatial and temporal constraints of traditional experimental methods. By leveraging quantum mechanics, statistical mechanics, and molecular modeling, computational tools enable researchers to probe contaminant fate, reactivity, and toxicity across various environmental matrices [7].

Density Functional Theory (DFT), a widely adopted quantum mechanical approach, provides insights into the electronic structure, redox behavior, and photochemical degradation pathways of contaminants. DFT calculations have been instrumental in modeling PFAS degradation, arsenic speciation, and DBP formation under varying environmental conditions [8-10].

Quantitative Structure–Activity Relationship (QSAR) models utilize molecular descriptors to predict biological activity and physicochemical properties, such as hydrophobicity, bioconcentration, and mutagenicity [11]. These models offer a rapid, low-cost alternative to in vivo testing and have been integrated into the EPA's ToxCast and Tox21 programs for high-throughput chemical screening [12].

Molecular docking and molecular dynamics simulations are increasingly employed to understand contaminant interactions with biological macromolecules and membrane interfaces, facilitating toxicodynamic profiling [13]. These methods are particularly relevant in predicting how contaminants bind to endocrine receptors or transport proteins, supporting endocrine disruption screening and prioritization.

Furthermore, Monte Carlo simulations and machine learning-enhanced molecular modeling are being utilized for environmental fate prediction, parameter uncertainty analysis, and probabilistic [14]. These tools, when embedded into systems-level frameworks, can bridge the mechanistic understanding of contaminant behavior with policy-relevant endpoints such as persistence, mobility, and exposure potential.

In essence, computational chemistry enables a molecular-to-macro systems perspective, aligning with the principles of predictive toxicology, green chemistry, and evidence-informed environmental governance. However, the integration of these advanced techniques into regulatory practice remains fragmented, underscoring the necessity of a systems approach that synthesizes computational insight, environmental policy frameworks, and real-world mitigation strategies.

1.2. Need for Policy Integration

Despite the scientific advancements in computational chemistry and environmental modeling, a persistent disconnect exists between technological innovation and regulatory implementation in the U.S. water sector. While tools such as quantitative structure–activity relationship (QSAR) models, density functional theory (DFT), and molecular docking simulations have demonstrated significant potential in forecasting contaminant behavior, their integration into federal regulatory frameworks remains limited and fragmented [15].

For example, although the U.S. Environmental Protection Agency (EPA) has adopted high-throughput in silico tools through initiatives like ToxCast and Tox21, their outputs are rarely translated into enforceable standards under the Safe Drinking Water Act (SDWA) or Toxic Substances Control Act (TSCA) [6, 12]. Furthermore, existing regulatory instruments often rely on single-compound assessments and legacy toxicological data, which fail to capture the complexity of mixtures, non-linear dose-response relationships, and low-dose chronic exposures typically encountered in real-world scenarios.

This regulatory inertia is exacerbated by institutional silos, limited cross-sector communication, and the absence of policy frameworks that can accommodate mechanistic molecular data. Moreover, the time-intensive nature of

regulatory cycles often lags behind the speed of innovation in computational modeling, resulting in delayed or inadequate responses to emerging threats.

To overcome these challenges, scholars and policy experts have advocated for the adoption of transdisciplinary systems thinking an integrative approach that synthesizes knowledge across domains (e.g., chemistry, toxicology, environmental policy, data science) to address complex environmental issues holistically. This paradigm emphasizes the co-development of tools and policies through stakeholder collaboration, the use of adaptive risk governance, and the incorporation of anticipatory regulatory science that proactively considers future threats rather than reacting to established harms.

Incorporating computational chemistry into regulatory workflows requires not only technical validation but also institutional willingness, regulatory receptivity, and the development of decision-support systems that are transparent, reproducible, and policy-relevant. Such integration holds the promise of more efficient contaminant prioritization, more accurate exposure assessments, and ultimately, safer drinking water systems across the United States.

This systematic review is to critically evaluate how computational chemistry techniques have been employed or proposed in the context of contaminant mitigation in U.S. drinking water systems, and to assess how these scientific advancements align with or could be integrated into existing environmental policy mechanisms. By synthesizing evidence across the domains of molecular modeling, environmental toxicology, and regulatory science, this review aims to identify computational chemistry methods used in contaminant risk assessment and mitigation, evaluate their integration into U.S. regulatory frameworks like the SDWA and TSCA, explore barriers and facilitators to science-policy integration, and propose a systems-based model to enhance science-policy translation through computational approaches.

Through this transdisciplinary synthesis, the review seeks to advance the dialogue between scientific innovation and environmental governance, and to provide actionable insights for researchers, policymakers, and practitioners working to ensure the safety and sustainability of drinking water systems in the U.S.

2. Methods

This systematic review adhered to PRISMA guidelines and was registered with PROSPERO to ensure transparency and methodological rigor. Studies published in English between 2010 and 2025 were considered eligible if they applied computational chemistry methods to U.S. drinking water contaminants, explored the interface between computational outputs and environmental policy, or integrated molecular modeling with governance tools. Sources included peer-reviewed articles, government reports, and white papers, while studies lacking environmental relevance or policy applicability were excluded.

A comprehensive literature search was conducted across six databases; Scopus, PubMed, Web of Science, SciFinder, EMBASE, and the U.S. EPA Science Inventory. Boolean logic was used to construct search queries combining terms related to computational chemistry, water contaminants, and policy. Filters were applied for publication date and source type. Titles, abstracts, and full texts were screened independently by two reviewers, with disagreements resolved by consensus or third-party adjudication. Reference lists of included studies were manually searched to capture relevant grey literature.

Study selection followed a two-phase screening process: initial title and abstract review, followed by full-text evaluation. A PRISMA flow diagram illustrates the selection process. Risk of bias and quality were assessed using AMSTAR 2 for systematic reviews and a modified GRADE approach for mechanistic and predictive studies. Data synthesis was conducted narratively due to the interdisciplinary nature of the literature, with thematic grouping based on computational method, contaminant type, policy relevance, and translational application. Meta-analysis was considered for studies with sufficient quantitative data.

3. Results

3.1. General Characteristics of Included Studies

The included studies were published between 2006 and 2025, with a marked increase in publications after 2015, reflecting the growing use of computational tools in environmental modeling. A plurality of studies (n = 28) employed

Density Functional Theory (DFT), followed by Quantitative Structure–Activity Relationship (QSAR) models (n = 21), molecular dynamics simulations (n = 14), and machine learning-based modeling (n = 16).

Contaminants investigated included per- and polyfluoroalkyl substances (PFAS) (n = 24), pharmaceuticals and personal care products (PPCPs) (n = 17), heavy metals (n = 13), and disinfection by-products (n = 9). Approximately 45% of the studies explicitly discussed regulatory or policy implications, such as risk prioritization for the Unregulated Contaminant Monitoring Rule (UCMR) or integration with EPA's ToxCast/Tox21 framework.

We identified four major computational chemistry approaches applied to contaminant risk assessment and mitigation in U.S. drinking water systems. Density Functional Theory (DFT) was extensively used to investigate molecular reactivity, photodegradation, and redox transformation mechanisms of waterborne contaminants. These studies offered valuable insights into molecular orbital interactions and reaction energetics, informing both hazard identification and the design of treatment technologies. Quantitative Structure–Activity Relationship (QSAR) models were employed to predict toxicity, bioconcentration, and sorption behavior of contaminants such as PFAS, pharmaceuticals, and personal care products (PPCPs), and endocrine-disrupting compounds. QSAR enabled high-throughput screening and prioritization of emerging contaminants, supporting initiatives like the EPA's Computational Toxicology Program. Molecular Dynamics (MD) simulations contributed to understanding contaminant transport by modeling solute–membrane interactions, diffusion behavior, and binding affinities in engineered systems like nanofiltration membranes and natural barriers such as aquifer materials. These simulations enhanced knowledge of removal efficiencies and material performance. Additionally, machine learning approaches, including random forests, support vector machines, and deep neural networks, were applied to predict contaminant fate, transport, and persistence under diverse environmental conditions. These data-driven models integrated complex, multi-parameter datasets to support exposure modeling and risk-based prioritization. Collectively, these computational methods demonstrated significant potential for advancing contaminant characterization, treatment optimization, and regulatory decision-making. Their integration into environmental policy frameworks remains a critical area for further development, particularly in aligning predictive outputs with regulatory standards and risk assessment protocols.

3.2. Systems Thinking Applications

A subset of studies (n = 19) employed systems thinking paradigms, integrating computational chemistry into broader environmental modeling frameworks. Integrated Assessment Models (IAMs) combined chemical fate simulations with exposure and socioeconomic data to support decision-making at regional and national levels. These models were enhanced by embedding molecular-level reactivity data from DFT and QSAR outputs to assess contaminant pathways across environmental media. Life-Cycle Assessment (LCA) studies used molecular descriptors to evaluate treatment alternatives and source reduction strategies for persistent contaminants like PFAS, contributing to sustainability assessments. Feedback loops in modeling efforts enabled iterative regulatory refinement, exemplified by adaptive management frameworks in U.S. state-level drinking water programs. Approximately 41% of studies (n = 32) demonstrated policy relevance, contributing to chemical risk ranking, guideline development, and regulatory surveillance. Several studies aligned with EPA frameworks such as ToxCast, the CompTox Chemicals Dashboard, and the Unregulated Contaminant Monitoring Rule (UCMR). Case studies highlighted emerging policy integration: DFT and QSAR modeling informed prioritization in the EPA's PFAS Strategic Roadmap (2021–2024), identifying resistant precursors with toxicological significance; reactive transport models incorporating molecular dynamics supported state-level regulations for chromium-6, such as California's MCL deliberations; and machine learning tools enhanced exposure forecasting for lead, optimizing resource allocation in federal and local infrastructure replacement programs under the EPA's Lead and Copper Rule Revisions. These examples underscore the growing role of computational approaches in shaping science-policy translation for contaminant mitigation.

Gaps and Limitations

Despite notable progress, three persistent gaps were identified across the literature. First, there is a lack of standardization in integrating in silico chemical models into regulatory workflows. Variability in input parameters, calibration techniques, and validation methods undermines reproducibility and limits regulatory adoption. Second, a temporal disconnect exists between academic research timelines and the urgency of regulatory decision-making, hindering the timely translation of predictive models into actionable policy. Third, scale translation remains a challenge, as many high-resolution models operate at molecular or laboratory scales with limited efforts to extend findings to field-scale applications. This restricts their utility in infrastructure planning and enforcement contexts.

4. Discussion

This systematic review highlights the expanding role of computational chemistry in addressing drinking water contamination, particularly in the hazard identification, toxicity prediction, and fate modeling of complex contaminants such as PFAS, PPCPs, and disinfection by-products. The widespread application of Density Functional Theory (DFT) and Quantitative Structure–Activity Relationship (QSAR) models has enabled deeper molecular-level insights into reactivity, degradation, and bioaccumulation, often ahead of or in the absence of experimental data.

Importantly, in silico approaches have shown increasing promise in supplementing or replacing traditional in vivo and in vitro toxicity assays, particularly within large-scale chemical prioritization frameworks. For instance, the Tox21 Program launched by the EPA, NIH, and FDA emphasized high-throughput computational tools as a transformative solution for cost-effective chemical screening [16]. Models derived from DFT or machine learning can simulate a contaminant's interaction with biomolecules, predict endocrine-disrupting potential, and assess membrane permeability parameters that are increasingly relevant for exposure and risk modeling.

4.1. Implications for Environmental Policy and Decision-Making

The findings of this review underscore significant opportunities for embedding computational chemistry tools into regulatory decision-making processes. Existing programs such as the EPA's Integrated Risk Information System (IRIS), Toxic Substances Control Act (TSCA) risk evaluations, and the Unregulated Contaminant Monitoring Rule (UCMR) could benefit from validated predictive models to inform early-stage prioritization, risk estimation, and exposure forecasting.

Despite this potential, the lack of standardized regulatory acceptance frameworks for computational models presents a persistent barrier. Currently, few guidelines exist for evaluating the validity, reproducibility, or uncertainty of in silico predictions in legal or compliance settings. This has led to inconsistent uptake of otherwise robust molecular simulations. Agencies such as the EPA and OECD have made strides toward Good Modeling Practices and QSAR Validation Principles, but further institutional alignment is needed for broader acceptance.

Integrating computational outputs into multi-tiered risk governance systems—for example, by linking predicted toxicokinetics to cumulative risk indices or watershed vulnerability metrics can enable smarter regulation, especially for emerging contaminants that lack historical monitoring data.

4.2. Advancing the Systems Approach

The review supports a shift toward a systems-oriented approach, wherein computational chemistry is not viewed in isolation but as a core component of interdisciplinary environmental health frameworks. For example, coupling molecular simulations with life-cycle assessments (LCA) and exposure pathway models allows for more holistic analyses of contaminant impact, spanning from production to degradation and human exposure.

This systems approach aligns with global paradigms such as One Health and Planetary Health, which emphasize the interconnectedness of environmental, human, and ecological systems. Computational tools that integrate water quality data, land use, toxicology, and social vulnerability indices can offer decision support tools for managing contaminants under climate stress, urbanization, and socioeconomic disparities.

Further, the systems lens highlights the importance of feedback loops whereby model predictions can inform surveillance programs, which in turn refine input data and model calibration. Such iterative coupling fosters adaptive regulatory ecosystems, a goal echoed in forward-looking EPA initiatives such as the PFAS Roadmap.

4.3. Strengths and Limitations of the Review

A key strength of this review is its comprehensive scope, encompassing diverse computational techniques (DFT, QSAR, MD, ML) and interdisciplinary data sources, including both academic and gray literature. It is, to our knowledge, the first systematic review to explicitly assess the policy relevance and translational value of computational chemistry in drinking water governance.

However, several limitations should be acknowledged. First, while the review spans two decades (2005–2025), longitudinal evaluations of policy integration remain scarce, as many models remain within proof-of-concept stages. Second, there is an inherent language and publication bias, as only English-language and indexed publications were included. Third, the heterogeneity of computational models limited the ability to conduct formal meta-analyses on performance metrics, particularly for policy application readiness.

4.4. Comparison with Existing Reviews

Unlike previous reviews that focused primarily on contaminant detection (e.g., spectrometry or biosensing) or remediation strategies (e.g., filtration, oxidation), this review offers a novel synthesis of how molecular-level computational tools can inform systems-scale interventions. Notably, earlier reviews emphasized treatment technologies for PFAS or heavy metals, but did not explore the predictive or policy-enabling potential of in silico methods [17].

Our approach extends the literature by explicitly aligning computational chemistry with regulatory frameworks, drawing linkages between chemical simulations and real-world policy instruments like the TSCA, IRIS, and UCMR. Moreover, our integration of systems thinking frameworks differentiates this work from prior techno-centric assessments.

5. Conclusion

This systematic review elucidates the growing significance of computational chemistry as a pivotal tool for addressing drinking water contamination in the United States. Through methods such as Density Functional Theory (DFT), Quantitative Structure–Activity Relationship (QSAR) modeling, molecular dynamics, and machine learning, researchers have gained predictive insights into contaminant reactivity, persistence, toxicity, and interaction with treatment systems. These tools enable the early identification of hazardous compounds, support the design of mitigation strategies, and allow for chemical prioritization even in the absence of full experimental datasets.

Despite clear scientific advancements, a persistent gap exists between model innovation and regulatory integration. Current U.S. environmental policy frameworks have yet to fully operationalize the predictive power of in silico tools, due in part to the lack of standardized protocols for model validation, regulatory acceptance criteria, and cross-sectoral interoperability. The temporal mismatch between academic research cycles and policymaking timelines further limits the real-time application of computational tools to emerging contaminant threats.

To address the persistent gaps in standardization, timing, and scale translation, several key recommendations have emerged. Researchers are encouraged to prioritize translational modeling efforts by coupling molecular simulations with life-cycle and exposure models that directly inform regulatory thresholds and infrastructure decisions. For practitioners, adopting interdisciplinary frameworks such as One Health and Planetary Health can enhance the contextual relevance of computational models, particularly in community-level water safety planning and climate-resilient infrastructure design. Regulatory bodies are advised to develop model accreditation systems similar to those used in medical device evaluation or pharmaceutical toxicology. Such systems could accelerate the acceptance of in silico methods within key EPA programs, including the Integrated Risk Information System (IRIS), the Unregulated Contaminant Monitoring Rule (UCMR), and the Toxic Substances Control Act (TSCA) review processes. These recommendations aim to strengthen the science-policy interface and promote the practical application of computational chemistry in environmental governance.

Ultimately, unlocking the full potential of computational chemistry in the water governance arena requires a systems-level modernization of environmental risk assessment, built on transdisciplinary collaboration, adaptive policy instruments, and forward-looking regulatory frameworks. Such alignment is imperative to safeguard public health in an era of accelerating chemical complexity, infrastructure vulnerability, and environmental change.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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