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Editorial

Characteristics of Impactful Computational Contributions to *The Journal of Physical Chemistry C*

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With the widespread availability of computational modeling tools and interest in computation-driven research, *The Journal of Physical Chemistry (JPC)* has received an increasing number of submissions of computation-focused manuscripts. That a contribution develops or applies computational tools is not in and of itself evidence of appropriateness for the Journal. The focus of *JPC* is on science that provides significant new physical insights or that presents new, general methods or tools that have the potential to lead to new physical insights in the broadly defined chemistry domain. It is thus timely to consider what constitutes evidence of physical insight or a new method in a primarily or exclusively computational contribution to the Journal. Given the breadth of the Journal and the diversity of physical chemistry, no one set of characteristics will apply to all contributions. Generally speaking, however, computational contributions to *JPC C* will have some substantial combination of the following attributes:

- **Relevance**: The work is motivated by a physical chemical problem of topical relevance to the Journal.

- **Significant physical insight**: The work provides and highlights physical insight that has a substantial and significant scope. These insights go beyond the computational prediction of the structural, electronic, mechanical, or chemical properties of a single system or a small number of systems. The insights are generalized and logically connected to the larger space of relevant systems. Insights into the physical origins of properties are provided.

- **Conceptual clarity**: The conceptual framework and the fundamental assumptions underlying the work are clearly laid out and placed into proper context.

- **Literature context**: The work appropriately summarizes and makes a critical comparison with related and relevant literature. It places the work in the proper context of the larger field. If the primary contribution is in predicting materials with a particular property, then a review of and a critical comparison with similar contributions is provided. That review and critical comparison highlights evidence that similar materials have been realized in the laboratory and that similar predictions have been verified in the experiment.

- **Experimental connection**: The work makes connections with, rationalizes, or aids in the interpretation of experimental observations. The work identifies the implications of the results for the problem of interest and suggests new experiments to validate predictions.

- **Appropriate model**: The work justifies the models. Computational models are frequently based on an idealization of a system as it would exist in the physical world, in the intended application. Impactful work considers and demonstrates that the model captures the salient features of the system relevant to the problem of interest and thus justifies the predictive merits of the work. In work that predicts new materials, appropriate evidence is provided that the material can exist as modeled under the conditions of the relevant application.

- **Substantial**: The work represents a significant, non-incremental advance on models that precede it.

- **Reproducible**: The work provides sufficient details, in the main text or in the Supporting Information, to allow other competent scientists to reproduce the reported results. These details include references to relevant software, a description of the theoretical models, delineation of the parameters relevant to the execution of those models, and a complete reporting of the model results. Results include, at a minimum, full reporting of structural information and numerical results relevant to further analysis, ideally in a machine-readable form. Representative input and output files are encouraged to be included in the Supporting Information. Authors are further encouraged to deposit all input, output, and analyses in a persistent repository that is accessible through a digital object identifier.

- **Robust**: The insights claimed from the work are demonstrated to be robust with respect to the computational models. Model approximations are articulated and validated either within the work itself or through reference to other efforts to validate. Electronic structure predictions are robust with respect to computational details (basis sets, reciprocal space sampling, system size, etc.), new force fields are validated using modern statistical approaches (cross-validation, etc.), and molecular dynamics/Monte Carlo simulations are statistically converged and are robust to minor changes in underlying potential.

- **New method**: Work that develops and/or applies a new computational methodology relevant to topical problems is appropriate for *JPC C*. New methodologies should be compared against and demonstrate advantages over existing models. New physical insights are preferred but are not a requirement of a contribution that reports the development of a new computational methodology. However, the motivation for that new development should be clearly described.
- **Benchmarking**: Works that benchmark computational models may be appropriate for *JPC*. That work must make close and critical comparisons with available experiments and/or with widely used comparable models. Works that highlight the physical origins of the varying performances of models are particularly desired.

In addition to these points specific to computational research, the most successful and impactful contributions will follow best practices in the preparation and reporting of results. Manuscript titles will appropriately capture the nature of the work, in particular, making clear the computational or predictive nature of the contribution. The abstract will appropriately summarize the approach and key results, and conclusions will emphasize the new physical insights provided by the work. Cover letters will direct editors toward that physical insight and its relevance to the Journal.

Computation has had a profound and positive impact on physical chemistry, and *The Journal of Physical Chemistry* is committed to being the venue of choice for publishing impactful, innovative, and physically insightful computational research. We thank our authors, reviewers, and readers for their invaluable and enduring contributions to realizing this vision.

For further insights into how editors make decisions regarding the appropriateness of a contribution to *The Journal of Physical Chemistry*, readers are invited to consult the Viewpoints on a variety of topical areas available in the New Physical Insights Virtual Issue. Additional information about criteria and preparation of submissions to *The Journal of Physical Chemistry* can be found in the Guidelines to Authors document.

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Notes