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Viewpoint

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New Physical Insights for Manuscripts on Organic and Perovskite-based Photovoltaics (and Other Optoelectronic Devices)

Something that may not be readily apparent to authors of manuscripts submitted to *The Journal of Physical Chemistry* (*JPC*) family of journals is that, as documented in our Information for Authors, the journal is no longer interested in publishing articles that are primarily focused on materials synthesis and characterization. There are many good materials-oriented venues in the literature, both within and external to the ACS family of journals, for this type of work, and the Editors felt that it was important that new research published in *JPC* contain significant new physical insights rather than a description of the synthesis and detailed characterization of new materials. This editorial shift has caused some confusion, particularly in communities where the new materials are characterized by employing them in optoelectronic devices, such as photovoltaics (PVs), light-emitting diodes (LEDs), memory elements, or field-effect transistors (FETs). Particularly prominent in this category are manuscripts dealing with organic bulk heterojunction and lead-halide perovskite-based PVs.

In the organic PV community, the Editors still receive numerous papers for consideration in *JPC* in which new semiconducting polymers or occasionally a new fullerene or other electron acceptor is synthesized, UV−vis and photoluminescence spectra of the new materials are reported, and the new materials are fabricated into a bulk heterojunction solar cell, with the open-circuit voltage, fill factor, and short-circuit current reported as well as possibly carrier mobilities or DFT calculations rationalizing the device performance. In the view of the *JPC* Editors, even though the new materials were used in an optoelectronic device or were the subject of quantum chemistry calculations, this class of manuscript falls squarely into the class of "materials synthesis and characterization"; device performance, without in-depth analysis, is simply another type of characterization. As a result, such manuscripts are generally rejected without review or are transferred to a more appropriate ACS journal in consultation with the authors. Even if a series of related polymers or electron acceptors is synthesized and the results are compared across the series, if the main point of the manuscript is the power conversion efficiency of the best material or best device geometry, then the Editors of *JPC* would still consider such a paper not to contain significantly new physical insights.

That said, there is a lot of good work in the organic PV community that is entirely appropriate for publication in *JPC*. For example, *JPC* Editors would likely send out for review papers in which a series of new materials is used to address the physics of how bulk heterojunction PV devices operate. For example, papers aimed at addressing morphology control and structure/function relationships affecting organic PV device performance, discussing the factors affecting exciton dissociation and polaron production such as energy level offsets, elucidating the roles of charge injection or collection at various interfaces, or examining what aspects of different materials control carrier mobilities or recombination are clearly appropriate subject material for *JPC* because they are focused on answering physically motivated questions and providing new physical insights. That said, *JPC* is less interested in papers in which some aspect of an organic PV device is changed and performance is improved but there is no real attempt at understanding the physics or physical chemistry behind the improvement. For example, papers utilizing new electron or hole transport or interfacial layers that enhance efficiency without additional measurements or calculations explaining why the enhancement occurs are likely to be rejected without review. Similarly, papers in which theoretical calculations are used to predict the performance of new materials that have not yet been synthesized and for which the theoretical methods have not been carefully benchmarked are also likely to be considered "virtual synthesis and characterization" and thus lacking in new physical insights. Of course, the above analysis also applies to manuscripts focused on materials for organic FETs, LEDs, and memory devices as well as for PVs and dye-sensitized solar cells (DSSCs).

The requirements for new physical insights are also similar for papers dealing with the properties of lead halide and other perovskite materials that have recently found their way into numerous optoelectronic devices and PVs in particular. PV power conversion efficiencies are particularly high for this class of materials, and there is much interest in improving efficiency and long-term stability of perovskite-based devices as well as in the fundamentals of how they operate. There are many fascinating questions concerning these materials, the answers to which will certainly play out in the pages of *JPC*. These include the role of grain boundaries in carrier mobility and device performance, the way composition and surface passivation affect the basic electronic properties of the material, the mechanisms by which carriers are transported or recombine, and the way ferroelectric properties of these materials affect their optoelectronic behavior, among many others. As with the organic PV work described above, papers that primarily focus on new procedures for producing perovskite films, the development of new surface passivators, and/or new hole transport layers that improve device performance but do not address the physics of why performance is improved will likely be rejected without review.

Overall, the re-engineering of optoelectronic devices of any kind that is not motivated by clear physical questions are papers that are clearly important to their field but that the Editors of *JPC* feel are better suited for another journal. As always, if you have any doubts as to whether a particular manuscript is appropriate for *JPC*, please feel free to contact any of the Senior Editors listed on the *JPC* Masthead for advice.

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Notes

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