CHEMISTRY OF MATERIALS

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Comments

Reply to Comment on "Environmental Stability of Crystals: A Greedy Screening"

Cite This: *Chem. Mater.* 2023, 35, 804−804

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Stability prediction is of great importance because it allows us to understand the behavior of materials under different conditions and to better assess how they will perform in relevant use cases. This information is crucial for the design and development of new materials, as well as for optimizing the performance of existing materials in a wide range of application areas.

In a comment on our article[1] on the stability screening of crystalline materials in an external environment using a heuristic greedy algorithm, Ai and Schrier[2] report an alternative approach that provides an exact solution to the problem in a time efficient manner. We are fully supportive of their study and highlight the following five points in response:

1. Stability is an important materials metric, both as a property to be predicted during inverse design and a down selection filter (refinement), as it focuses limited experimental bandwidth on the most promising target compounds with greatest likelihood to be synthesized (reduces false positives).
2. Decomposition prediction presents a promising path worth exploring for materials stability prediction. There is interest to develop stability prediction tools that do not require calculation of the entire phase diagram, to rapidly predict the stability of any given compound under realistic and relevant conditions. Decomposition predictors are one such a pathway, whereby the likelihood of a given compound to decompose into other compounds is estimated.
3. These developments represent an open access win. We are happy to see alternative approaches for decomposition prediction proposed by other authors, stimulated by result of our recent paper. We are also impressed that these results came quickly, within a few months between preprint publication posting, because the code was available as open access through a GitHub repository. This is a big win for open access and also for *Chemistry of Materials* for facilitating the scientific discourse.
4. Ai and Schrier's comment is an interdisciplinary win. At its essence, decomposition prediction in its current form is a search process. Ai and Schrier did well to leverage experience in other fields, including mathematics, allowing more efficient algorithms that can be transferred and adapted to materials chemistry needs. Other approaches to the heuristic greedy search, including direct methods proposed by the authors or a bloom filter-based search, may be more appropriate as materials databases expand in number of entries and approach those of proteomics.
5. Remaining challenges for decomposition prediction include a strategy for when the relevant data concerning a decomposition product is not available in the database, and thus cannot be looked up (e.g., an underexplored region of composition or a highly competitive non-crystalline phase), as well a more complete description of the atomic chemical potentials at finite temperatures and pressures.[3] These require further developments, including effective search and optimization strategies where an exact solution is no longer possible.

In conclusion, the linear optimization approach for the identification of oxidation products described by Ai and Schrier shows that there are viable alternatives to being greedy when seeking solutions to materials stability and design problems.

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Notes

The authors declare no competing financial interest.

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Received: December 5, 2022
Published: January 11, 2023