Towards a Roadmap of Chemical Space

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The "chemical space" concept refers to the set of all solids and molecules across compositional and configurational space. In practice, limited subsets of chemical space are usually defined according to some boundary conditions. This can be a trivial task (e.g. for all binary octet semiconductors) or require significant effort (e.g. for all organic molecules up to a certain size). To date, research in this field is mostly concerned with enumerating the components of a subset of interest and finding correlations between properties (e.g. structure-property relationships). The purpose of this contribution is to shift the focus from individual compounds to chemical reactions. This means that chemical space is transformed from a list of compounds to a network of reactions connecting them (i.e. a map).

This higher degree of organization has significant benefits for benchmarking and parameterizing semiempirical electronic structure approaches. Using a dataset of ~11,000 reaction energies, we show that the common practice of benchmarking methods against atomization energies does not allow strong conclusions about how the performance for reaction energies.[1] Reaction based alternatives are discussed.

The reaction-based mapping of chemical space also has important implications for data-driven chemical research. We will show how the space of chemical reactions can be constructed and organized in a systematic and exhaustive manner. This enables the discovery of new chemistry and the elucidation of reaction meachanisms.[2]

[1] J. T. Margraf, D. S. Ranasinghe and R. J. Bartlett, *Phys. Chem. Chem. Phys.* **2017**, 19, 9798–9805.

[2] J. T. Margraf, K. Reuter, *in preparation*.