A generalized many-body expansion and a unified view of fragmentation methods in electronic structure theory

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Fragment-based quantum chemistry methods have emerged as a promising route to reducing the high cost of *ab initio* electronic structure calculations in large systems. Recent work has concluded that all fragment based approaches can be uniquely defined by specifying: a fragment creation algorithm, if and how interactions with other fragments are accounted for, and the expansion for the property of interest. This last item needs to be specified because the expansion explicitly depends on whether or not the fragments intersect (*i.e.* have common atoms). Here we derive a general many-body expansion for intersecting fragments; this expansion, reduces to the expansion for non-intersecting fragments if the fragments are forbidden from intersecting. In addition to unifying the intersecting and non-intersecting cases, this expansion also presents the first straightforward method for introducing energy corrections due to higher ordered unions of intersecting fragments, allowing for systematic improvement of the predicted energy for intersecting fragments in the same way as for non-intersecting fragments. In light of this new expansion, we also reevaluate what key elements are necessary to specify an fragment based approach and conclude that the specification of: a fragmentation algorithm, a method for dealing with severed valencies, a method to account for fragment-fragment interactions, and the number of layers (in an ONIOM sense) is sufficient.

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