Exactly Embedded Density Functional Theory for Modeling Chemical Reactions

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We will describe embedded density functional theory methods for performing accurate and scalable electronic structure theory calculations in large molecular systems [1,2], with application to clusters, liquids, and electrode interfaces.

[1] Goodpaster JD, Ananth N, Manby FR, and Miller TF, *J. Chem. Phys.*, **133**, 084103 (2010).
[2] Goodpaster JD, Barnes TA, and Miller TF, *J. Chem. Phys.*, **134**, 164108 (2011).