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Abstract for an Invited Paper
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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 (2010) 084103.
[2] Goodpaster JD, Barnes TA, and Miller TF, J. Chem. Phys., 134 (2011) 164108.