

Abstract Submitted
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Hartree-Fock and Kohn-Sham method for open systems YONGXI ZHOU, MATTHIAS ERNZERHOF, University of Montreal — The source-sink potential (SSP) method [1,2] provides a simple description of electron transport through molecules. Starting from the tight-binding approach, the infinite contacts are replaced by complex potentials. Extending SSP, we describe how to introduce complex potentials into the Hartree-Fock and the Kohn-Sham method. Doing so enables us to model open systems with a current passing through, while accounting for exchange and correlation effects. The implementation of these methods and initial results will be discussed.

- [1] F. Goyer, M. Ernzerhof, M. Zhuang, J. Chem. Phys. 126, 144104 (2007).
[2] M. Ernzerhof, J. Chem. Phys. 127, 204709 (2007).

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