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Dissociation of diatomic molecules and the exact-exchange Kohn-Sham potential: the case of LiF ADI MAKMAL, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel, STEPHAN KUEMMEL, Physikalisches Institut, Universitat Bayreuth, D-95440 Bayreuth, Germany, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — The incorrect fractional-charge dissociation of stretched diatomic molecules, predicted by semi-local exchange-correlation functionals, is revisited. This difficulty can be overcome with asymptotically correct non-local potential operators, but should also be absent in exact Kohn-Sham theory, where the potential is local. Here, we show, for the illustrative case of the LiF dimer, that the exact-exchange local Kohn-Sham potential, constructed within the Krieger, Li, and Iafrate (KLI) approximation, can lead to binding energy and charge dissociation curves that are qualitatively correct. This correct behavior is traced back to a characteristic "step" structure in the local exchange potential and its relation to the Kohn-Sham eigenvalues is analyzed.

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