

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Examining the role of pseudopotentials in exact-exchange-based Kohn-Sham gaps ADI MAKMAL, Weizmann Institute of Science, Israel, RICKARD ARMIENTO, Universitaet Bayreuth, Germany, EBERHARD ENGEL, Goethe-Universitaet Frankfurt, Germany, LEEOR KRONIK, Weizmann Institute of Science, Israel, STEPHAN KUEMMEL, Universitaet Bayreuth, Germany — We present exact-exchange optimized effective potential calculations of the Kohn-Sham gap, using highly accurate grid-based all-electron and pseudopotential approaches for prototypical diatomic molecules. Results obtained with pseudopotentials that have been constructed in a manner consistent with the exact-exchange functional agree with the all electron results for the cases studied. This confirms the reliability of the pseudopotential approximation for orbital-dependent functionals such as exact exchange.

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Date submitted: 20 Nov 2009

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