

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

**Gentlest Ascent Dynamics for Calculating First Excited State
and Exploring Energy Landscape of Kohn-Sham Density Functionals**

CHEN LI, JIANFENG LU, WEITAO YANG, Duke University — We develop the gentlest ascent dynamics (GAD) for Kohn-Sham density functional theory to search for the index-1 saddle points (*i.e.*, the stationary points with one and only one energy descending direction) on the energy landscape of the Kohn-Sham density functionals. These stationary solutions correspond to excited states in the ground state functionals. As shown by various examples, the first excited states of many chemical systems are given by these index-1 saddle points. Our novel approach provides an alternative, more robust way to obtain these excited states, compared with the widely used Δ SCF approach. The method can be easily generalized to target higher index saddle points. Our results also reveal the physical interest and relevance of studying the Kohn-Sham energy landscape.

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Date submitted: 04 Nov 2015

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