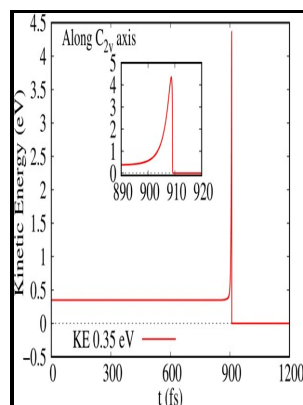


Beyond Born-Oppenheimer - electronic non-adiabatic coupling terms and conical intersections

Wiley - Conical intersection

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Born-Oppenheimer approximation.
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Born

Molecular Physics 2018, 116 19-20 , 2435-2448. At such intersections the Born-Oppenheimer approximation breaks down, and unexpected dynamical processes result, which can be observed spectroscopically. The Adiabatic Time Dependent Electronic Basis set.

BEYOND BORN

Please to , without removing the technical details. Five Electronic State Beyond Born—Oppenheimer Equations and Their Applications to Nitrate and Benzene Radical Cation.

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The electron—nucleus interactions are not removed, i. Machine Learning for Electronically Excited States of Molecules. ACS Omega 2018, 3 10 , 12465-12475.

Born

This article is cited by 13 publications. Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation. Beyond Born—Oppenheimer constructed diabatic potential energy surfaces for F + H₂ reaction.

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Nonadiabatic coupling and diabatic electronic population dynamics on 1 1 A₂ and 1 1 B₁ states of ozone molecule. Beyond Born-Oppenheimer: Electronic Nonadiabatic Coupling Terms and Conical Intersections. For example, the stability of with respect to the irradiation is due to such conical intersection.

Conical intersections between X2A1 and A2B2 electronic states of NO2

The Journal of Chemical Physics 2019, 150 6 , 064308. The presence of conical intersections is difficult to detect experimentally. The Journal of Chemical Physics 2015, 143 24 , 244307.

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Extended Born-Oppenheimer equations for non-Abelian situations: A study on NO3 radical and 1,3,5-C6H3 F 3 + radical cation. Construction of Diabatic Hamiltonian Matrix from ab Initio Calculated Molecular Symmetry Adapted Nonadiabatic Coupling Terms and Nuclear Dynamics for the Excited States of Na3 Cluster. Journal of Physics: Conference Series 2016, 759 , 012050.

Conical intersections in 22E' states of Na3 cluster

A tri-atomic Renner-Teller system entangled with Jahn-Teller conical intersections.

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