

Publications

Direct non-Born-Oppenheimer variational calculations of all bound vibrational states corresponding to the first rotational excitation of D₂ performed with explicitly correlated all-particle Gaussian functions.

K.L. Sharkey; [N.Kirnosov](#); L. Adamowicz. JOURNAL OF CHEMICAL PHYSICS Volume: 142 Article Number: 174307, Published: MAY 7 2015

Para-ortho isomerization of H₂⁺. Non-Born-Oppenheimer direct variational calculations with explicitly correlated all-particle Gaussian functions

[N.Kirnosov](#); K.L. Sharkey; L. Adamowicz.

CHEMICAL PHYSICS LETTERS Volume: 621, Pages 134-140, Published: FEB 4 2015

A comparison of two types of explicitly correlated Gaussian functions for non-Born-Oppenheimer molecular calculations using a model potential

M. Formanek, K. L. Sharkey, N. Kirnosov and L. Adamowicz

JOURNAL OF CHEMICAL PHYSICS Volume: 141 Article Number: 54103 Published online: OCT 15 2014

Charge asymmetry in the rovibrationally excited HD molecule

[N.Kirnosov](#); K.L. Sharkey; L. Adamowicz.

JOURNAL OF CHEMICAL PHYSICS Volume: 140 Issue: 10 Article Number: 104115 Published online: MAR 13 2014

Lifetimes of rovibrational levels of HD⁺

[N.Kirnosov](#); K.L. Sharkey; L. Adamowicz.

PHYSICAL REVIEW A Volume: 89 Issue: 1 Article Number: 012513 Published: JAN 27 2014

Charge asymmetry in rovibrationally excited HD⁺ determined using explicitly correlated all-particle Gaussian functions

[N.Kirnosov](#); K.L. Sharkey; L. Adamowicz. JOURNAL OF CHEMICAL PHYSICS Volume: 139 Issue: 20 Article Number: 204105 Published: NOV 28 2013

An algorithm for non-Born-Oppenheimer quantum mechanical variational calculations of N=1 rotationally excited states of diatomic molecules using all-particle explicitly correlated Gaussian functions

K.L. Sharkey; [N.Kirnosov](#); L. Adamowicz. JOURNAL OF CHEMICAL PHYSICS Volume: 139 Issue: 16 Article Number: 164119 Published: OCT 28 2013

Non-Born-Oppenheimer method for direct variational calculations of diatomic

first excited rotational states using explicitly correlated all-particle Gaussian functions

K.L. Sharkey; N.Kirnosov; L. Adamowicz. PHYSICAL REVIEW A Volume: 88 Issue: 3
Article Number: 032513 Published: SEP 20 2013

Analytical energy gradient used in variational Born-Oppenheimer calculations with all-electron explicitly correlated Gaussian functions for molecules containing pi electrons.

W.-C. Tung; M. Pavanello; K.L. Sharkey; N.Kirnosov; L. Adamowicz. JOURNAL OF CHEMICAL PHYSICS Volume: 138 Issue: 12 Article Number: 124101 Published: MAR 28 2013

An algorithm for quantum mechanical finite-nuclear-mass variational calculations of atoms with $L=3$ using all-electron explicitly correlated Gaussian basis functions

K.L. Sharkey; N.Kirnosov; L. Adamowicz. JOURNAL OF CHEMICAL PHYSICS Volume: 138 Issue: 10 Article Number: 104107 Published: MAR 14 2013