SELECTED RECENT PUBLICATIONS

SERGEI MANZHOS AND TUCKER CARRINGTON JR.,
“Using rectangular collocation with finite difference derivatives to solve electronic Schrödinger equation”,

XIAO-GANG WANG AND TUCKER CARRINGTON JR.,
“Computing tunnelling splittings of HOD dimer”,
Physical Chemistry Chemical Physics xxx, yyy-zzz (2018)

ERIC TOOMBS AND TUCKER CARRINGTON,
“Redundant Coordinates in Quantum Mechanics”,

PHILLIP S. THOMAS, TUCKER CARRINGTON, JAY AGARWAL
HENRY F. SCHAEFER III,
“Using an iterative eigensolver and intertwined rank reduction to compute vibrational spectra of molecules with more than a dozen atoms: uracil and naphthalene”,
Selected as “Featured Article”,

A.J. BARCLAY, A.R.W. MCKELLAR, K.H. MICHAELIAN, N. MOAZZEN-AHMADI, RICHARD DAWES,
XIAO-GANG WANG, AND TUCKER CARRINGTON JR.,
“Infrared spectrum and potential energy surface of the CO-O2 dimer”,
Physical Chemistry Chemical Physics 20, 14431--14440 (2018)

HUBERT CYBULSKI, CHRISTIAN HENRIKSEN, RICHARD DAWES, XIAO-GANG WANG, NEHA BORA, GUSTAVO AVILA, AND TUCKER CARRINGTON JR., BERTA FERNANDEZ,
“Ab initio study of the CO-N2 complex: A new highly accurate intermolecular potential energy surface and rovibrational spectrum”,
Physical Chemistry Chemical Physics 20, 12624 – 12636 (2018)

TUCKER CARRINGTON JR.,
“Iterative methods for computing vibrational spectra”,
Mathematics, 6, 13-1 – 13-14 (2018) [190]

XIAO-GANG WANG AND TUCKER CARRINGTON JR.,
“A numerically exact full dimensional calculation of rovibrational levels of water dimer”,

ROBERT WODRASZKA AND TUCKER CARRINGTON,
"A new collocation-based multi-configuration time-dependent Hartree (MCTDH) approach for solving the Schroedinger equation with a general potential energy surface”,
Selected as Editor’s Pick,

ZHIQIANG ZHAO, JUN CHEN, ZHAOJUN ZHANG, DONG H. ZHANG, XIAO-GANG WANG, TUCKER CARRINGTON JR., AND FABIEN GATTI,
“Full-dimensional calculations of rovibrational levels of five-atom molecules using two different strategies: Applications to CH₄, CHD₃, CH₃D and CH₃F”,

J. NOROOZ OLIAEE, N. MOAZZEN-AHMADI, A.R.W. MCKELLAR, XIAO-GANG WANG, AND TUCKER CARRINGTON JR.,
“The He₂ - OCS complex: comparison between theory and experiment”,

SERGEI MANZHOS, XIAO-GANG WANG, AND TUCKER CARRINGTON JR.,
“A multimode-like scheme for selecting the centers of Gaussian basis functions when computing vibrational spectra”,
Chem. Phys. 509, 139-144 (2018) [Hans-Dieter Meyer Festschrift]

PUSHP BAJAJ, XIAO-GANG WANG, TUCKER CARRINGTON JR., FRANCESCO PAESANI,
Selected as Editor’s Pick,

ADITYA KAMATH, RODRIGO VARGAS-HERNÁNDEZ, ROMAN V. KREMS, TUCKER CARRINGTON, AND SERGEI MANZHOS,
Selected as Editor's Pick,

GUSTAVO AVILA AND TUCKER CARRINGTON JR.,
“Computing vibrational energy levels of CH₄ with a Smolyak collocation method”,
J. Chem. Phys. 147, 144102-1 – 144102-10 (2017) [182]

GUSTAVO AVILA AND TUCKER CARRINGTON JR.,
“Reducing the cost of using collocation to compute vibrational energy levels: results for CH₃NH”,

GUSTAVO AVILA, JENS OETTERSHAGEN, AND TUCKER CARRINGTON JR.,
“Comparing nested sequences of Leja and PseudoGauss points to interpolate in 1D and solve the Schroedinger equation in 9D”,

ROBERT WODRASZKA AND TUCKER CARRINGTON,
“Systematically expanding nondirect product bases within the pruned multi-configuration time-dependent Hartree (MCTDH) method: A comparison with multi-layer MCTDH”,

PHILLIP S. THOMAS, AND TUCKER CARRINGTON,
“An intertwined method for making low-rank, sum-of-product basis functions that makes it possible to compute vibrational spectra of molecules with more than 10 atoms”,

TUCKER CARRINGTON JR.,
“Computing (ro-)vibrational spectra of molecules with more than four atoms”,
TUCKER CARRINGTON JR.,
“Using iterative eigensolvers to compute vibrational spectra”,

XIAO-GANG WANG AND TUCKER CARRINGTON JR.,
“Using monomer vibrational wavefunctions as contracted basis functions to compute rovibrational levels of an H2O-atom complex in full dimensionality”,

SERGEI MANZHOS AND TUCKER CARRINGTON,
“Using an internal coordinate basis and a space-fixed Cartesian coordinate kinetic energy operator to compute a vibrational spectrum with Gaussian basis functions and rectangular collocation”,

EDUARDO CASTRO, GUSTAVO AVILA, SERGEI MANZHOS, JAY AGARWAL, HENRY F. SCHAEFFER III, AND TUCKER CARRINGTON JR.,
“Using a new neural-network potential and a sparse-grid collocation method to compute the vibrational spectrum of phosgene”,

ARNAUD LECLERC, PHILLIP S. THOMAS, AND TUCKER CARRINGTON,
“Comparison of different eigensolvers for calculating vibrational spectra using low-rank, sum-of-product basis functions”,

JAMES BROWN AND TUCKER CARRINGTON,
“Using an expanding nondirect product harmonic basis with an iterative eigensolver to compute vibrational energy levels with as many as seven atoms”,

GUSTAVO AVILA AND TUCKER CARRINGTON JR.,
“Pruned bases that are compatible with iterative eigensolvers and general potentials: new results for CH3CN”,
Chem. Phys. 482, 3-8 (2017) (Lenz Cederbaum Festschrift) [170]

XIAO-GANG WANG, TUCKER CARRINGTON, AND RICHARD DAWES,
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ROBERT WODRASZKA AND TUCKER CARRINGTON,
“Using a pruned nondirect product basis in conjunction with the multi-configurational time-dependent Hartree (MCTDH) method”,

JAMES BROWN AND TUCKER CARRINGTON,
“Assessing the utility of phase-space-localized basis functions: exploiting direct product structure and a new basis function selection procedure”,

GEOFF DONOGHUE, XIAO-GANG WANG, RICHARD DAWES, AND TUCKER CARRINGTON, JR.

M.DEHGHANY, MOJTABA REZAEI, N. MOAZZEN-AHMADI, A.R.W. MCKELLAR, JAMES BROWN, XIAO-GANG WANG, AND TUCKER CARRINGTON, JR.

XIAO-GANG WANG AND TUCKER CARRINGTON JR.,
“Calculated rotation-bending energy levels of CH$_5$” and a comparison with experiment”,
Selected by AIP journal editors as paper of great interest

STEVE NDENGUÉ, RICHARD DAWES, XIAO-GANG WANG, TUCKER CARRINGTON JR., ZHIGANG SUN, AND HUA GUO,
“Calculated Vibrational States of Ozone up to Dissociation”,

ARNAUD LECLERC AND TUCKER CARRINGTON JR.,
“Using symmetry-adapted optimized sum-of-products basis functions to calculate vibrational spectra”,

PHILLIP S. THOMAS, TUCKER CARRINGTON JR.,
“Using nested contractions and a hierarchical tensor format to compute vibrational spectra of molecules with seven atoms”,

SERGEI MANZHOS, TUCKER CARRINGTON JR., LAURA LAVERDURE, NICHOLAS MOSEY
“Computing the Anharmonic Vibrational Spectrum of UF$_6$ in 15 Dimensions with an Optimized Basis Set and Rectangular Collocation”,

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JAMES BROWN AND TUCKER CARRINGTON JR.,
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“The vibration-rotation-tunneling levels of N$_2$-H$_2$O and N$_2$-D$_2$O”,

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“Two new methods for computing vibrational energy levels”,


TAPTA KANCHAN ROY, TUCKER CARRINGTON JR., AND R. BENNY GERBER, “Approximate First-Principles Anharmonic Calculations of Polyatomic Spectra Using MP2 and B3LYP Potentials: Comparisons with Experiment”,

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