SELECTED RECENT PUBLICATIONS

JONAS KU, ADITYA KAMATH, TUCKER CARRINGTON, SERGEI MANZHOS.
“Machine learning optimization of the collocation point set for solving the electronic Schrödinger equation”,

EMIL ZAK AND TUCKER CARRINGTON JR,
“Using collocation and a hierarchical basis to solve the vibrational Schroedinger equation”,

ROBERT WODRASZKA AND TUCKER CARRINGTON JR,
"Efficiently transforming from values of a function on a sparse grid to basis coefficients”,

ROBERT WODRASZKA AND TUCKER CARRINGTON JR,
"A pruned collocation-based multi-configuration time-dependent Hartree approach using a Smolyak grid for solving the Schroedinger equation with a general potential energy surface”,
Selected as Editors Pick,

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”,

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”,
Selected as HOT article.


GUSTAVO AVILA AND TUCKER CARRINGTON JR.,
“Reducing the cost of using collocation to compute vibrational energy levels: results for CH₂NH”,

GUSTAVO AVILA, JENS OETTERSHAGEN, AND TUCKER CARRINGTON JR.,
“Comparing nested sequences of Leja and PseudoGauss points to interpolate in 1D and solve the Schrödinger 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. SCHAEFER 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 CH$_3$CN”，
Chem. Phys. 482, 3-8 (2017) (Lenz Cederbaum Festschrift) [170]

XIAO-GANG WANG, TUCKER CARRINGTON, AND RICHARD DAWES,
“Computational Study of the Rovibrational Spectrum of (CO$_2$)$_2$”，

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.
“Computational Study of the Rovibrational Spectra of CO$_2$-C$_2$H$_2$ and CO$_2$-C$_2$D$_2$”，

M.DEHGHANY, MOJTABA REZAEI, N. MOAZZEN-AHMADI, A.R.W. MCKELLAR, JAMES BROWN, XIAO-GANG WANG, AND TUCKER CARRINGTON, JR.
“Intermolecular vibrations of the CO$_2$ – CS$_2$ complex: Experiment and theory agree, but understanding remains challenging”，

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”,

GUSTAVO AVILA AND TUCKER CARRINGTON JR.,
“A multi-dimensional Smolyak collocation method in curvilinear coordinates for computing vibrational spectra”,

JAMES BROWN AND TUCKER CARRINGTON JR.,
“Using an iterative eigensolver to compute vibrational energies with phase-spaced localized basis functions”,

XIAO-GANG WANG AND TUCKER CARRINGTON JR.,
“The vibration-rotation-tunneling levels of N₂-H₂O and N₂-D₂O”,

TUCKER CARRINGTON JR.,
“Two new methods for computing vibrational energy levels”,
Canadian Journal of Chemistry 82, 900-914 (2015)

MOUMITA MAJUMDER, SAMUEL E. HEGGER, RICHARD DAWES, SERGEI MANZHOS, XIAO-GANG WANG, TUCKER CARRINGTON JR., JUN LI, AND HUA GUO,
“Explicitly-correlated MRCI-F12 potential energy surfaces for methane fit with several permutation invariant schemes and full-dimensional vibrational calculations”,

GUSTAVO AVILA AND TUCKER CARRINGTON JR.,
“Using multi-dimensional Smolyak interpolation to make a sum-of-products potential”,

TUCKER CARRINGTON JR.,
“New methods for computing ro-vibrational energy levels”,

S. MANZHOS, R. DAWES, AND T. CARRINGTON JR.,
“Neural Network Based Approaches for Building High Dimensional and Quantum Dynamics-Friendly Potential Energy Surfaces”,

TUCKER CARRINGTON JR.,
“Methods for computing ro-vibrational energy levels”,

JAMES BROWN AND TUCKER CARRINGTON JR.,
“Comment on "Phase-Space Approach to Solving the Time-Independent Schroedinger Equation””,

XIAO-GANG WANG AND TUCKER CARRINGTON JR.,
“Using experimental data and a contracted basis Lanczos method to determine an accurate methane potential energy surface from a least squares optimization”,
XIAO-GANG WANG AND TUCKER CARRINGTON JR.,
“Ro-vibrational levels and wavefunctions of ClH₂O”,

ARNAUD LECLERC AND TUCKER CARRINGTON JR.,
“Calculating vibrational spectra with sum of product basis functions without storing full-dimensional vectors or matrices”,

JAMES BROWN, XIAO-GANG WANG, TUCKER CARRINGTON JR., G. S. GRUBBS II, AND RICHARD DAWES
“Computational study of the rovibrational spectrum of CO2-CS2”,

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”,