IMLS Publications

Gia G. Maisuradze and Donald L. Thompson,  
(Part of the special issue “Donald J. Kouri Festschrift”)  

Gia G. Maisuradze, Donald L. Thompson, Albert F. Wagner, and Michael Minkoff,  

Akio Kawano, Yin Guo, Donald L. Thompson, Albert F. Wagner, and Michael Minkoff,  
“Improving the Accuracy of Interpolated Potential Energy Surfaces by Using an Analytical Zeroth-Order Potential Function,”  

Yin Guo, Akio Kawano, Donald L. Thompson, Albert F. Wagner, and Michael Minkoff,  

Gia G. Maisuradze, Akio Kawano, Donald L. Thompson, Albert F. Wagner, and Michael Minkoff,  
“Interpolating Moving Least-Squares Methods for Fitting Potential Energy Surfaces: Analysis of an Application to a Six-Dimensional System"  

Donald L. Thompson, Albert F. Wagner, and Michael Minkoff,  
“Advanced Computational Methods for Simulating Chemical Reactions,”  

Igor V. Tokmakov, Saman Alavi, and Donald L. Thompson,  
“Urea and Urea Nitrate Decomposition Pathways: A Quantum Chemistry Study,”  

Akio Kawano, Igor V. Tokmakov, Donald L. Thompson, Albert F. Wagner, and Michael Minkoff,  

Donald L. Thompson, Albert F. Wagner, and Michael Minkoff,  
“Advanced Computational Methods for Simulating Chemical Reactions,”  
Yin Guo, Lawrence B. Harding, Albert F. Wagner, Michael Minkoff, and Donald L. Thompson,
“Interpolating Moving Least-Squares Methods for Fitting Potential Energy Surfaces: An Application to the H$_2$CN Unimolecular Reaction,”

Richard Dawes, Donald L. Thompson, Yin Guo, Albert F. Wagner, and Michael Minkoff,
“Interpolating Moving Least-Squares Methods for Fitting Potential Energy Surfaces: Computing High-Density PES Data from Low-Density \textit{ab initio} Data,”

Igor Tokmakov, Albert F. Wagner, Michael Minkoff, and Donald L. Thompson,
“Gradient incorporation in one-dimensional applications of interpolating moving least-squares methods for fitting potential energy surfaces,”

Yin Guo, Igor Tokmakov, Donald L. Thompson, Albert F. Wagner, and Michael Minkoff,

Richard Dawes, Donald L. Thompson, Albert F. Wagner, and Michael Minkoff,

Richard Dawes. Alessio Passalacqua, Albert F. Wagner, Thomas D. Sewell, Michael Minkoff, and Donald L. Thompson,

Jon P. Camden, Richard Dawes, and Donald L. Thompson,
“Application of Interpolating Moving Least Squares (IMLS) Fitting to Hypervelocity Collision Dynamics: O($^3P$) + HCl,”

Richard Dawes, Albert F. Wagner, and Donald L. Thompson,
“\textit{Ab Initio} Wavenumber Accurate Spectroscopy: $^1$CH$_2$ and HCN Vibrational Levels on Automatically Generated IMLS Potential Energy Surfaces”