DUAN, FRANK XIAOFENG:

Dr. Duan has a wide scientific background and twenty-eight-year experience applying supercomputer technology to solve research problems in physics, chemistry and material science. Dr. Duan's research includes studying SiC clusters using Density Functional Theory and adapting the Nuclear-Electron Orbital codes to calculate positron and muon wavefunctions. He currently works as a senior computer scientist managing and supporting computational chemistry applications at AFRL DSRC. He has been an Adjunct Associate Professor since 2011 in Dept. of Engineering Physics, AFIT.

<xiaofeng.duan.ctr@us.af.mil>

Recent Relevant Publications

1. "The Closo-Si12C12 Molecule from Cluster to Crystal: Effects of Hydrogenation and Oligomerization on Near-Optical Excited States" Xiaofeng F. Duan, and Larry W. Burggraf, J. Chem. Phys. 146, 234302 (2017)
2. "Ab Initio Calculations for e+e- Contact Density of Positrons Interacting with Diatomic and Polyatomic Molecules" W.K.I.L.Wanniarachchi, C.G. Morgan, G. Kedziora, H.B. Schlegel, X. Duan, L. Burggraf, M. Pak, in preparation
3. "Predictive coupled-cluster isomer orderings for some SinCm (m, n ≤ 12) clusters: A pragmatic comparison between DFT and complete basis limit coupled-cluster benchmarks" J.N. Byrd, J.J. Lutz, Y. Jin, D.S. Ranasinghe, J.A. Montgomery Jr., A. Perera1, X.F. Duan, L.W. Burggraf, B.A. Sanders and R.J. Bartlett, J. Chem. Phys. 145, 024312 (2016)
4. "The closo-Si12C12 molecule from cluster to crystal: A theoretical prediction", Xiaofeng F. Duan and Larry W. Burggraf, J. Chem. Phys. 144, 114309 (2016)
5. "Theoretical Investigation on Optical Properties of Si12C12 Clusters" Xiaofeng F. Duan and Larry W. Burggraf, J. Chem. Phys. 142, 034303 (2015)
6. "Searching for Stable SinCn Clusters: Combination of Stochastic Potential Surface Search and Pseudopotential Plane-Wave Car-Parinello Simulated Annealing Simulations" Xiaofeng F. Duan, Larry W. Burggraf, and Lingyu Huang, Molecules 2013, 18, 8591-8606