

## Publications (Sudha Srinivas)

1. Silver and Gold mediated nucleobase bonding, S. Srinivas, P. H. Acioli, K Vogleonsger, N. Nicholson, J. Hibdon, N. Wrinkle, and D. Rutschman, Proceedings of the Eighth Annual Mentoring Institute Conference, editor N. Dominguez, pg. 1154-1157 (University of New Mexico, 2015).
2. Silver and Gold mediated nucleobase bonding, P. H. Acioli and S. Srinivas, Journal of Molecular Modeling 20, 2391 (2014).
3. Experiential Learning of Classical Mechanics Through Molecular Dynamics, P. H. Acioli and S. Srinivas, Proceedings of the World Conference on Physics Education, Istanbul, Turkey, editor M. Taşar, p 385-396 (Pegem Akademi, 2013).
4. An Exploration of the Potential Energy Surface of Ag<sub>7</sub>CO, P. H. Acioli, S. Burkland, and S. Srinivas, European Physical Journal D 66, 215 (2012).
5. Density functional Theory study of Ag-Cluster/CO Interactions, P. H. Acioli, N. Ratanavade, M. R. Cline, and S. Srinivas, Lecture Notes in Computer Science, Springer Verlag (Heidelberg), Vol. 5545, 203 (2009).
6. Atomistic Description of Electric Dipole Polarizability in Si<sub>n</sub>H<sub>m</sub>, S. Srinivas, M. Yang, K. Jackson, and J. Jellinek, Comp. Meth. Sci. and Eng. 1108, 71 (2009).
7. A Density-Functional Study of the Structure and Self-Organization in Spin Clusters, S. Srinivas and E. Torikai, Journal of Magnetism and Magnetic Materials, Vol. 310, 2390 (2007).
8. Structure, Bonding and Magnetism in Manganese Clusters, P. Bobadova-Parvanova, K. A. Jackson, S. Srinivas and M. Horoi, Journal of Chemical Physics, Vol. 122, 014310 (2005)
9. First-principles investigations of the Structural and Electronic Properties of Small Beryllium Clusters, S. Srinivas and J. Jellinek, Journal of Chemical Physics, Vol. 121, 7243 (2004)
10. Emergence of antiferromagnetic ordering in Mn clusters, P. Bobadova-Parvanova, K. A. Jackson, S. Srinivas and M. Horoi, Phys. Rev. A 67, 61202 (2003)
11. Density-functional investigations of the spin ordering in Fe<sub>13</sub>clusters, P. Bobadova-Parvanova, K. A. Jackson, S. Srinivas, and M. Horoi, Physical Review B Vol. 66, 195402 (2002)
12. Modeling the <sup>119</sup>Sn Mossbauer Spectra of Chalcogenide Glasses using Density Functional Theory Calculations, K. Jackson, S. Srinivas, J. Kortus and M. Pederson, Physical Review B, Vol. 65, 214201 (2002)
13. Scanning the Potential Energy Surface of Iron Clusters: Novel Search Strategy, P. Bobadova-Parvanova, K. Jackson, S. Srinivas, M. Horoi, C. Köhler and G. Seifert, Journal of Chemical Physics, Vol. 116, 3576 (2002)
14. Theoretical Investigations of the Interaction of Silver Trimer with Ethylene Molecule, U. A. Salian, S. Srinivas and J. Jellinek, Chemical Physics Letters, Vol. 345, 312 (2001)
15. The interaction of Ammonia with small iron clusters: Infrared spectra and density functional calculations of Fe<sub>n</sub>(NH<sub>3</sub>)<sub>m</sub> complexes, K. A. Jackson, M. B. Knickelbein, G. Koretsky and S. Srinivas, Chemical Physics, Vol. 262, 41 (2000)
16. Ab Initio Monte Carlo Investigations of Li Clusters, Sudha Srinivas and J. Jellinek, Physica Status Solidi, Vol. 217, 311 (2000)
17. Theoretical Investigations of Silver Clusters and Silver Ligand Systems, Sudha Srinivas, Umesh Salian and J. Jellinek, NATO Advanced Study Institute (ASI) Series on Metal-Ligand

- Interactions in Chemistry, Physics, and Biology, published by Kluwer Academic Publishers, Dordrecht, Netherlands (1999)
18. Ab Initio Monte Carlo: Application to Li<sub>8</sub>, Julius Jellinek, Sudha Srinivas and Piercarlo Fantucci, Chemical Physics Letters, Vol. 288, 705 (1998)
  19. Theory of Hyperfine Interactions Associated with the Negative Muon in Lanthanum Copper Oxide High T<sub>c</sub> System, Sudha Srinivas, S.B.Sulaiman, N. Sahoo, T.P. Das, E. Torikai, K. Nishiyama and K. Nagamine, Hyperfine Interactions, Vol. 105, 167 (1997)
  20. Probing Interaction of Paramagnetic Electron with Conduction Electron in High T<sub>c</sub> Superconductor LaSrCuO by ( $\mu^-$ O) Spin Relaxation, E. Torikai, K. Nagamine, K. Nishiyama, E. Hirose, Y. Ikedo, T. Hashimoto, P. Birrer, I. Tanaka, H. Kojima, S. Srinivas, T.P. Das, S. Maekawa, K. Yamada, and Y. Endoh, Hyperfine Interactions, Vol. 105, 175 (1997)
  21. Ab Initio Investigations on Sb<sub>4</sub> Analogous Zintl Clusters, F. Hagelberg, Sudha Srinivas, N. Sahoo, T.P. Das and K.G. Weil, Physical Review A, Vol. 53, 353 (1996)
  22. Interaction of Paramagnetic Electron with High T<sub>c</sub> Supercurrent in La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> studied by Negative Muon Probe, E. Torikai, K. Nagamine, K. Nishiyama, E. Hirose, P. Birrer, I. Tanaka, H. Kojima, S. Srinivas, T.P. Das and S. Maekawa, Hyperfine Interactions, Vol. 97-98, 387 (1996)
  23. Theory of Nuclear Quadrupole Interactions in Solid Fluoromethanes with Implanted <sup>19</sup>F\* Nuclei: Coupling of HF\* and Host Molecule, G. Gowri, T. Briere, S. Srinivas, T.P. Das, M. Frank and W. Kreishe, Zeitschrift Fur Naturforschung A, Vol. 51, 565 (1996)
  24. First-Principles Investigation of Nitrogen Nuclear Quadrupole Interactions in the RDX (C<sub>3</sub>H<sub>6</sub>N<sub>6</sub>O<sub>6</sub>) System, Ranjit Pati, Sudha Srinivas, T. Briere, N. Sahoo, T.P. Das and S. N. Ray, Journal of Physical Chemistry, Vol. 99, 9051 (1995)
  25. First Principles Investigation of <sup>19</sup>F\* Nuclear Quadrupole Interaction in IV Group Tetrafluorides, H.S. Cho, T. Briere, S. Srinivas, C. Russel, G. Gowri, R. Pati, T.P. Das, M. Frank, W. Kreishe and K. B. Nielsen, Hyperfine Interactions, Vol. 96, 213 (1995)
  26. Theory of the Location and Associated Hyperfine Properties of the Positive Muon in La<sub>2</sub>CuO<sub>4</sub>, S.B. Sulaiman, Sudha Srinivas, N. Sahoo, F. Hagelberg, T.P. Das, E. Torikai and K. Nagamine, Physical Review B, Vol. 49, 9879 (1994)
  27. Theory of the Location and Associated Hyperfine Properties of the Positive Muon in La<sub>2</sub>CuO<sub>4</sub>, S.B. Sulaiman, N. Sahoo, Sudha Srinivas, F. Hagelberg, T.P. Das, E. Torikai and K. Nagamine, Hyperfine Interactions, Vol. 84, 87 (1994)
  28. Location and Associated Hyperfine Properties of  $\mu^+$  in La<sub>2</sub>CuO<sub>4</sub>, S.B. Sulaiman, N. Sahoo, Sudha Srinivas, F. Hagelberg, T.P. Das, E. Torikai and K. Nagamine, Hyperfine Interactions, Vol. 79, 901 (1993)
  29. Local Hyperfine Field Vector of Positive Muon in Mono-Domain Single Crystal of Antiferromagnetic La<sub>2</sub>CuO<sub>4</sub>, E. Torikai, H. Ishihara, K. Nagamine, H. Kitazawa, I. Tanaka, H. Kojima, S.B. Sulaiman, S. Srinivas and T.P. Das, Hyperfine Interactions, Vol. 79, 915 (1993)
  30. Behavior of Positive Muons in High T<sub>c</sub> Superconductors La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub>, E. Torikai, K. Nagamine, H. Kitazawa, I. Tanaka, H. Kojima, S.B. Sulaiman, S. Srinivas and T.P. Das, Hyperfine Interactions, Vol. 79, 921 (1993)
  31. Momentum Density and Fermi Surface of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>, R. Prasad and Sudha Srinivas Physica C, Vol. 162-164, 1335 (1989). Proceedings of the International Conference on High Tc Superconductivity, Stanford, CA (July 1989)