Dr. Muhammad Shabbir

Research area;

Computational study of electro-optical functional materials using different higher level quantum chemical methods. The study of photo-physical, optical and nonlinear optical properties is our main area of interest.

Key words;

Quantum chemistry, First and Second hyperpolarizabilities, open-shell molecules

Employment experience;

November,2010 – Present: Specially Appointed Assistant Professor, GCOE. Professor Masayoshi Nakano's laboratory, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan.

Education;

June 2004: M.Sc. in chemistry from University of Agriculture Faisalabad, Pakistan.
September 2007: Chinese proficiency language course from Northeast Normal University, P.R. China.
June 2010: Ph.D. in Physical Chemistry from Northeast Normal University, P.R. China.

Awards;

Award of cultural exchange scholarship for Ph.D. supported by both the Ministry of education Pakistan and China scholarship council.

Best poster award in 27th congress of Chinese Chemical Society held in 20-23 June 2010, Xiamen, China.

Selected publications;

1. *Shabbir Muhammad,* Hongliang Xu, Yi Liao, kan Yuhe, Zhongmin Su "Quantum Mechanical Design and Structure of Li@B10H14 Basket with Remarkably Enhanced Electro-Optical Response **J. Am. Chem. Soc. 2009**, *131* (33), 11833–11840.

2. *Shabbir Muhammad*, Muhammad Ramzan Saeed Ashraf Janjua, Zhongmin Su Investigation of dibenzoboroles having π-electrons: Towards a new type of two dimensional NLO molecular switch? **J. Phys. Chem. C, 2009**, *113*, 12551–12557.

3. *Shabbir Muhammad*, Chunguang Liu, Liang Zhao, Shuixing Wu, Zhongmin Su "A theoretical investigation of intermolecular interaction of a phthalimide based "on–off" sensor with different halide ions: tuning its efficiency and electro-optical properties." **Theor. Chem. Account, 2009,** 122, pp 77-86

4. *Shabbir Muhammad*, Hongliang Xu, Zhongmin Su "A Quantum Chemical Study of Benzimidazole Containing Molecules to Tune the Nonlinear Optical Switching by Proton Abstraction." **Phys. Chem. Chem. Phys., 2010,** 12(18): 4791-99.

5. *Shabbir Muhammad*, Hongliang Xu, Zhongmin Su "Capturing a Synergistic Effect of a Conical Push and an Inward Pull in Fluoro Derivatives of Li@B10H14 Basket: Toward a Higher Vertical Ionization Potential and Nonlinear Optical Response" **J. Phys. Chem. A, 2011**,DOI: 10.1021/jp110401f.

Research Statement;

In the modern optical communication systems, the fast replacement of electron by photon as a carrier of information has kept the design of different types of nonlinear optical (NLO) materials in the spotlight of scientific interest. Ab initio methods together with finite field (FF) approach are usually used to compute first and second hyperpolarizabilities, β and γ, which are the origins of the macroscopic second- and third-order nonlinear optical (NLO) susceptibilities, χ^2 and χ^3, respectively. Some recent studies have shown that few classes of push-pull NLO chromophores containing an electron donor, a conjugated (pi) network, and an electron acceptor are good single-molecule labels. Thus, NLO chromophores are potential candidates for designing reversibly switchable nanoscale emitters not only for single-molecule optical imaging in living cells but also for NLO microscopy. Near-infrared or nonlinear NLO chromophores have several advantages over visible fluorophores,

including improved tissue penetration, a significant ground-state dipole moment, sensitivity to local environment and lower auto-fluorescence for example indocyanine green. In the present study, a molecular-level description about these NLO chromophores will be provided which can revolutionize the field.

My goal;

Recently, Nakano et al. have reported that open-shell molecular systems can exhibit larger third- order NLO properties than closed-shell systems. According to this guideline, our goals include selection and modification of different recent computational methodologies to study the second-/third-order NLO properties using a more accurate, concise and detailed way in photolytic radicals, single wall carbon nanotubes, and open-shell compounds which have been considered a complicated task due to the multireference (MR) character of wave function in computational chemistry. Besides this, the use of different modified and selected methodologies to design new families of NLO chromophores, which have been considered difficult to deal in experimental chemistry due to high reactivity of open shell radicals. **The long-term goal** includes the continued development of high performance NLO chromophores and to modulate reversibly their second-order polarizability (by light and pH) and third-order polarizability (by change in spin state, charge state, applying external static field). **The future outlook** includes the designing of switchable NLO chromophores along with the elucidation of their integration mechanism to help in understanding their environmental sensitivity for imaging of single molecules.