Shehryar Khan

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Selected Competencies

Relativistic Quantum Theory	Ab-initio Molecular Dynamics
Density Functional Theory (DFT)	Nuclear Magnetic Resonance (NMR)
Wave-function methods	Spin-Orbit Coupling

Education

Stockholm University, Stockholm, Sweden, ***Sep '13 – Jun '18***
Doctor of Philosophy (PhD), Theoretical Chem. Physics

Uni. Groningen, Groningen, The Netherlands, ***Sep '11 – Aug '13***
Master of Science (MSc), Theoretical Chemistry and Computational Modeling

Toyama University, Toyama, Japan ***Apr '07 – Mar '11***
Bachelor of Engineering (BEng), Mechanical and Intellectual Systems Engineering

Osaka University of Foreign studies, Osaka, Japan ***Apr '06 – Mar '07***
Japanese Language Proficiency Certification

Scholarships and Awards

MARIE CURIE ITN Fellowship, European Union ***Sep '13 – Sep'16***
ERASMUS MUNDUS Scholarship, European Union ***Dec '11 – Aug'13***
MONBUKAGAKUSHO Scholarship, Japanese Government ***Apr `06 – Apr `11***

Work/Research Experience

SynCat, Synfuels China Lab. For Fundamental Research, Beijing, China ***Mar'19 – present***
Research collaboration: Application of machine-learning methods applied to calculations from Density Functional Theory (DFT) in condensed matter systems.

Department of Chemical Physics (DCP), Stockholm, Sweden ***Sep'13 – Jun '18***
Theoretical and computational investigations using relativistic quantum chemistry and (ab-initio) molecular dynamics simulations to study both static and dynamic electronic and magnetic properties of lanthanide complexes.

GIOTTO Biotech, Florence, Italy ***Jan'16-Jun'16***
Gained experience in experimental methods in the Nuclear Magnetic Resonance (NMR) laboratory of Prof. Giacomo Parigi and Prof. Claudio Luchinat. Computational studies related to calculating the magnetic susceptibility using first principles were also undertaken.

Slovak Academy of Sciences (SAS), Bratislava, Slovakia ***Jun'14- Sep'14***
Worked on applications of the 4-component relativistic Density Functional Theory (DFT) in-house software "ReSpect" with the group of Prof. Vladimir Malkin.

Laboratoire de Chemie et Physique Quantique(LCPQ), Toulouse, France ***Feb'13–Jun' 13***
Worked under Prof. Fabienne Alary to perform ab-initio studies of transition metal complexes relevant for solar cell applications. The calculations involved use of Natural Bond Order (NBO) analysis and time-dependant density functional theory (TD-DFT) to calculate photophysical and photochemical properties.

Department of Theoretical Chemistry (DTC), Groningen, The Netherlands ***Sep'11 – Aug'13***

Worked under Prof. Ria Broer with various theoretical and computational methods in chemistry and physics.

Applied Mechano-Informatics Laboratory (AMIL), Toyama, Japan ***Apr '10 – Apr '11***

Worked under Prof. Zolotoukihina Tatiana on chemical kinetic and molecular dynamic simulations of hydrocarbons undergoing combustion during an ignition reaction. Principal author for research paper entitled "Molecular Dynamics of n-heptane oxidation reaction mechanism" published in the 50th National Heat Transfer Symposium Journal of Japan.

Publications

'Probing the photophysical capability of mono and bis(cyclometallated) Fe(II) polypyridine complexes using ground state DFT and TDDFT', I. M. Dixon, S. Khan, F. Alary, Boggio-Pasqua, and J.-L. Heully, *Dalton Transactions , Sep 2014*

'Systematic Theoretical Investigation of the Zero-Field Splitting in Gd(III) Complexes: Wave Function and Density Functional Approaches', S.Khan, A. Kubica, D.Kruk, J. Kowalewski and M. Odelius, *J. Chem. Phys., Jan 2015*

'An ab initio CASSCF study of Zero Field Splitting Fluctuations in the Octet Ground State of Aqueous [Gd(III)(HPDO3A)(H_2O)]' S.Khan, R. Pollet, R. Vuilleumier, J. Kowalewski, M. Odelius, *J. Chem Phys., Dec 2017*

'Zero-field splitting in the isoelectronic aqueous Gd(III) and Eu(II) complexes from a first principles analysis.' S.Khan, V. Peters, J. Kowalewski and M. Odelius, *Chem. Phys., Feb 2018*

Title of PhD Thesis: "Combined Quantum Mechanical and Molecular Dynamics study of paramagnetic complexes"

Computational Software

Programming/Scripting Languages:	Fortran77, Python, Octave, bash
Molecular Dynamics:	GROMACS, CPMD
Quantum-Chemistry:	GAMESS-UK, GAUSSIAN, ORCA, CP2K
Solid-state:	VASP/Quantum Espresso (Basic familiarity)
Machine-Learning:	Keras, Tensorflow, scikit-learn

Languages

English, Urdu, Japanese