

Dr. ANAND RAJKAMAL

Vellore, Tamilnadu, India.

rajkamalloyola@gmail.com

Skype No: 8489657980

Contact No: +82 010-2501-1988



Research Experience

2020/Sep-Till now Post-Doctoral Fellow, Department of Energy Science and Technology, Environmental Waste Recycle Institute, Myongji University, Yongin, Gyeonggi-do, 17058, Republic of Korea.

2018/June-2020/Aug Post-Doctoral Fellow, Chemical engineering department, IIT Bombay, India.

Research work

1. Solid electrolyte interphase layer and Cathode material in the lithium-ion batteries
2. Bimetallic Nanoparticle catalysts for CO oxidation

2014/Jan–2018/May Ph.D., Department of Physics, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamilnadu, India.

Thesis Title “CARBON ALLOTROPES AS ANODE MATERIALS FOR LITHIUM ION BATTERY”

Supervisors : Dr. Kathirvel, Assistant prof., Department of Physics, SRM Institute of Science and Technology

Co-Supervisor : Dr. Ranjit Thapa, Associate prof., Research Institute, SRM Institute of Science and Technology

Education

2009 – 2011 **M.Sc. in Physics**
Loyola college, Chennai, Tamilnadu, India.
Percentage obtained: 62.4%

2005 – 2008 **B.Sc. in Physics**
Voorhees College, Vellore, Tamilnadu, India.
Percentage obtained: 60.2%

Broad area of Research

- ❖ Computational Materials Science

Area of Research Interest

- ❖ Carbon based anode material for Lithium-ion battery
- ❖ Electrode/Electrolyte interface in the Lithium-ion battery
- ❖ Hydrogen storage, Catalyst (ORR, COR)
- ❖ Organic Light Emitting Diode

Computational Skills

DFT based codes: **Quantum ESPRESSO**, **VASP** and **Gaussian**

Molecular Dynamics Package: **GROMACS**

1. Ground-state calculations and Structural Optimization.

- ❖ Separable Norm-conserving and Ultrasoft (Vanderbilt) pseudo-potentials, PAW (Projector Augmented Waves);
- ❖ Several exchange-correlation functionals: from LDA to generalized-gradient corrections (PW91, PBE, B88-P86, BLYP) to meta-GGA, exact exchange (HF) and hybrid functionals (PBE0, B3LYP, HSE);
- ❖ VdW corrections (DFT-D) or nonlocal vdW functionals (vdw-DF, DF2, optpbe, optB88-vdW and optB86b-vdW);

2. Transition states and minimum energy paths.

- ❖ Nudged Elastic Band method

3. Molecular Dynamics

- ❖ Classical Molecular Dynamics – MD simulation, Umbrella Sampling Method
- ❖ Born-Oppenheimer Molecular Dynamics

4. Response properties (DFPT)

- ❖ Phonon frequencies and Full phonon dispersions

SKILLS FROM THE DFT CALCULATIONS

- ❖ Electronic Band Structure and Density of States (DOS)
- ❖ Orbitals Occupancy
- ❖ Charge Density Difference
- ❖ Projected Density of States
- ❖ Electron Localization Function (ELF)
- ❖ Nudged Elastic Band method
- ❖ Open Circuit Voltage
- ❖ Volume Expansion
- ❖ Formation Energy
- ❖ Phonon dispersion band structure and DOS
- ❖ AIMD
- ❖ Classical MD

TOOLS FOR MODELLING: **Materials Studio, VESTA, Avogadro, Xcrysden and VMD**

Awards and achievements

09- 11 Dec, 2016 **Best poster presentation award** *“Si doped T6 carbon: a promising anode material for Li-ion batteries with better stability and high storage capacity* on “The Indian science congress association-Chennai chapter”, Organized by SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamilnadu, India.

22-24 Sep, 2016 Our group conducted ‘**Asian Consortium on Computational Materials Science**’ Theme meeting on First-Principles Analysis & Experiment: Role in Energy Research, SRM Science and Technology, Chennai, India.

List of Publications

1. **A. Rajkamal**, Ranjit Thapa, “Carbon Allotropes as Anode Material for Lithium-Ion Batteries”, *Advanced Materials Technologies*, 4 (10), 1900307, (2019), 1-20 **IF: 7.84**
2. Paramita Banerjee, Ranjit Thapa, **A. Rajkamal**, K.R.S. Chandrakumar, G.P. Das “First-principles identification of the origin for higher activity of surface doped carbon nanohorn: Impact on hydrogen storage”, *International Journal of Hydrogen Energy*, 44 (41), 23196-23209 **IF: 5.81**
3. **A. Rajkamal**, S. Sinthika, Gunther Andersson, & Ranjit Thapa, Ring type and π electron occupancy of C atom decides the Li-ion storage properties of Phagraphene: An example of sp^2 hybridized C structure, *Carbon*, 129, (2018), 775–784, **IF: 9.59**
4. E. Mathan Kumar, **A. Rajkamal** and Ranjit Thapa, “Screening based approach and dehydrogenation kinetics for MgH_2 : Guide to find suitable dopant using First-principles approach”, *Scientific reports*, 7, (2017), 15550, **IF: 4.37**
5. S. Nandhini[#], **A. Rajkamal**[#], Biswajit Saha & Ranjit Thapa, “First- Principles identification of site dependent activity of graphene based electrocatalyst”, *Journal of Molecular Catalysis A-Chemical*, 432, (2017), 242–249 **IF: 5.06**, [#] same contribution
6. **A. Rajkamal**[#], E. Mathan Kumar[#], V. Kathirvel, Noejung Park & Ranjit Thapa, “Si doped T6 carbon structure as an anode material for Li-ion batteries: An ab initio study”, *Scientific reports*, 6, (2016), 37822. **IF: 4.37**, [#] same contribution
7. Ankur Sharma, **A Rajkamal**, *et al.*, “Addressing the High-Voltage Structural and Electrochemical Instability of Ni-Containing Layered Transition Metal (TM) Oxide Cathodes by Blocking the TM-Migration Pathway in the Lattice”, *ACS Applied Materials Interfaces* 13, (2021), 25836–25849. **IF: 9.23**
8. Erwin C Escobar, John Edward L Sio, Khino J Parohinog, **Anand Rajkamal**, *et al.*, “Hyper-crosslinked tetraphenylborate as a regenerable sorbent for Cs^+ sequestration in aqueous media through cation- π interactions”, *Chemosphere* 228, (2021), 132501. **IF: 7.08**

Conference Presentation

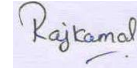
1. **A. Rajkamal**, V. Kathirvel, Ranjit Thapa, “Li adsorption and diffusion on 3D metallic T6 Carbon: First Principles study”, **Oral Presentation**, (15-17 Dec, 2015): *5th International Conference on Advances in Energy Research (ICAER-2015)*, Organized by IIT-Bombay, India.
2. **A. Rajkamal**, E. Mathan Kumar, V. Kathirvel, Noejung Park and Ranjit Thapa, “Si doped T6 carbon: a promising anode material for Li-ion batteries with better stability and high storage capacity”. **Poster Presentation**, (09 – 11 Dec, 2016): *The Indian science congress association-Chennai chapter Organized by SRM IST*, Kattankukathur, Chennai, India.
3. **Anand Rajkamal and Hern Kim** “Thermally Activated Delayed Fluorescence Host for High Performance Organic Light Emitting Diodes” **Poster Presentation**, (20 – 22 Oct, 2021): *Polymer Society's Fall Meeting*, Gyeongju HICO, South Korea.

Personal Information

Father's Name : Anand
Mother's Name : Padmini
Date of Birth : 19/03/1988
Gender : Male
Nationality : Indian
Languages Known : Tamil, English and Hindi.

I hereby declare that all the details furnished above are true to the best of my knowledge.

2021/Oct/24
Vellore-632002



(A. Rajkamal)