Arpan Kundu, PhD

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EDUCATION

Humboldt-Universität zu Berlin **Berlin, Germany**

Ph. D. (with "summa cum laude") in physical and theoretical chemistry April 2018

Thesis: Ab initio prediction of isotherms for pure and mixed gas adsorption in metal-organic frameworks.

Adviser: Prof. Joachim Sauer

Indian Institute of Technology (IIT) Kanpur **Kanpur, India**

M.Sc in Chemistry (GPA 9.7/10, 1st rank) May 2011

Thesis: Dynamical behavior of supercritical aqueous solutions: orientational motion and angular jumps.

Adviser: Prof. Amalendu Chandra

Jadavpur University **Kolkata, India**

B.Sc with honours in Chemistry (1st class with distinction, Marks 77.7%, 6th rank) May 2009

RESEARCH INTERESTS

- Development and application of *ab initio* methods for (i) electron-phonon interactions in materials; (ii) spin-phonon interactions in solid-state spin defects, (iii) catalysis and gas conversion technologies.

RESEARCH EXPERIENCE

University of Chicago, Pritzker School of Molecular Engineering (PME) **Chicago, IL, USA**

Staff Scientist, PI: Prof. Giulia Galli May 2024 – Present

Post doctoral scholar, Adviser: Prof. Giulia Galli Feb 2019 – Apr 2024

- Developed Molecular dynamics and stochastic methods, for electron-phonon interactions from first principles.
- Developed a python interface for coupling (i) i-PI: an universal force engine and (ii) Qbox: an efficient DFT solver.
- Developed a python package named PyEPFD for performing electron-phonon calculations.
- Machine learning interatomic potentials and materials' properties.

Humboldt-Universität zu Berlin, Institute für Chemie **Berlin, Germany**

Ph.D student and post doctoral researcher, Adviser: Prof. Joachim Sauer Nov 2012 – Jan 2019

- Development of an ab initio methodology for the prediction of pure and mixed gas adsorption in porous solids using quantum chemistry and statistical mechanics.
- Development of a FORTRAN package: LGCMC for simulating pure and mixed gas adsorption isotherm using grand canonical Monte Carlo simulations on a coarse-grained lattice of adsorption sites.

Indian Institute of Science, Solid State and Structural Chemistry Unit **Bangalore, India**

Research fellow Aug 2011 – July 2012

- Investigation of transport of water molecules within carbon nanotubes using force field based MD simulations.

Indian Institute of Technology (IIT) Kanpur, Department of Chemistry **Kanpur, India**

M.Sc project student Jan 2011 – Apr 2011

- Investigation of orientational relaxation and hydrogen bond breaking dynamics of supercritical water and aqueous solutions using force field based MD simulations.

Indian Institute of Technology (IIT) Kharagpur, Department of Civil Engineering **Kharagpur, India**

Summer research student May 2010-July 2010

- Wet synthesis of As^0 and Au^0 nanoparticles (of tunable dimension) and their application in surface-enhanced Raman scattering (SERS).

PUBLICATIONS

*** = Corresponding Author**

1. Berrens, M, **Kundu, A.,** Calegari-Andrade, M. F., Anh-Pham, T., Galli, G., Donadio, D.* "Nuclear quantum effects on the electronic structure of water and ice", *In Revision*, Preprint: arXiv:2405.06207.

2. Kundu, A.*, Galli, G.* "Quantum vibronic effects on the excitation energies of the nitrogen-vacancy center in diamond", *J. Phys. Chem. Lett.* **2024**, 15, 802, Preprint: arXiv:2401.06745. (co-corresponding author)

3. Kundu, A.*, Galli, G.* "*Quantum vibronic effects on the electronic properties of molecular crystals*", *J. Chem. Theory Comput.* **2023**, 19, 13, 4011. (co-corresponding author).

4. Sillar, K.*, **Kundu, A.***, Sauer. J. "*Ab initio prediction of adsorption selectivities for binary gas mixtures on a heterogeneous metal-organic framework surface*", *J. Phys. Chem. C* **2023**, 127, 27, 13317. (co-corresponding author)

5. Yang, H., Govoni, M.*, **Kundu, A.**, Galli, G.* *" Computational protocol to evaluate electron-phonon interactions within density matrix perturbation theory*", *J. Chem. Theory Comput.* **2022**, 18, 10, 6031.

6. Kundu, A.*, Song, Y., Galli, G.* **"***Influence of nuclear quantum effects on the electronic properties of amorphous carbon*", Proc. Natl. Acad. Sci. **2022**, 119, 31, e2203083119. (co-corresponding author),
Highlighted on PME News: "*A new look at disordered carbon*" by Sarah C. P. Williams.

7. Francese, T., **Kundu, A.**, Gygi, F., Galli, G.* "*Quantum simulations of thermally activated delayed fluorescence in an all-organic emitter*" *Phys. Chem. Chem. Phys.* **2022**, 24, 10101 .

8. Yang, H., Govoni, M.*, **Kundu, A.**, Galli, G.* "*Combined first-principles calculations of electron-electron and electron-phonon self energies in condensed systems*" *J. Chem. Theory Comput.* **2021**, 17, 12, 7468.

9. Kundu, A.*, Govoni, M., Yang, H., Ceriotti, M., Gygi, F., Galli, G.* "*Quantum vibronic effects on the electronic properties of solid and molecular carbon*" *Phys. Rev. Materials **2021**, 5, L070801*. (co-corresponding author)

10. Kundu, A.†, Sillar†, K., Sauer, J.* "*Predicting adsorption selectivities from pure gas isotherms for gas mixtures in metal-organic frameworks*" *Chem. Sci.* **2020**, 11, 643 (Featured in front cover).

11. Kundu, A., Sillar, K., Sauer, J.* "*Ab initio prediction of adsorption isotherms for gas mixtures by grand canonical Monte Carlo on a lattice of sites*" *J. Phys. Chem. Lett* **2017**, 8, 2713.

12. Sillar, K.*, **Kundu, A.**, Sauer. J. *"Ab initio adsorption isotherms for molecules with lateral interactions: CO_2 in metal-organic framework"* *J. Phys. Chem. C* **2017**, 121, 12789.

13. Kundu, A., Piccini, G., Sillar, K., Sauer, J.* *"Ab initio prediction of adsorption isotherms for small molecules in metal-organic frameworks"* *J. Am. Chem. Soc.* **2016**, 138, 14047.

14. Pal, A.*, Saha, S., Maji, S. K., Sahoo, R., Kundu, M., **Kundu, A.** *"Galvanic replacement of As(0) nanoparticles by Au(III) for nanogold fabrication and SERS application",* *New J. Chem.* **2014**, 38, 1675.

15. Pal, A.*, Saha, S., Maji S. K., Kundu, M., **Kundu, A.** *"Wet chemical synthesis of spherical arsenic nanoparticles by a simple reduction method and its characterization"*, *Adv Mat. Lett.* **2012**, 3, 177.

AWARDS AND ACADEMIC ACHIEVEMENTS

- Fischer-Nernst award 2018 for best Ph.D. thesis, Department of Chemistry, HU Berlin — Nov 2019
- Successfully defended funding (2 × 2 years) from German Science Foundation. — Nov 2013 – Oct 2017
- IMPRS Ph.D. scholarship, FHI Berlin — Nov 2012 – Oct 2013
- Shyama Prasad Mukherjee Fellowship (SPMF), CSIR: Govt. of India. — Sep 2011
- The proficiency medal for best M.Sc. project work, IIT Kanpur. — May 2011
- The general proficiency medal for best academic performance in M.Sc, IIT Kanpur. — May 2011
- All India 1st rank in "National Eligibility Test (NET)" examination conducted by CSIR, Govt. of India. — Dec 2010
- All India 11th rank in "Joint Admission test for M.Sc (JAM)" examination conducted by IITs. — May 2009

TEACHING/ MENTORING EXPERIENCE

University of Chicago, Pritzker School of Molecular Engineering (PME) **Chicago, IL, USA**

- Mentoring 1 master's and 2 grad students — December 2022 - Present
- Mentored an undergraduate researcher — June 2020 – Oct 2021

Humboldt-Universität zu Berlin **Berlin, Germany**

- Taught physical Chemistry 2: a practical course for master's students. — Summer 2015, summer 2016
- Taught Molecular Modelling (MoMo): a practical course for bachelor's students. — Summer 2013
- Supervised a visiting master's student researcher**.** — Summer 2013

CONFERENCES/WORKSHOPS

Invited and contributed talks

- **Kundu, A.**, Galli, G. "*Quantum nuclear vibrations and electronic properties of molecular crystals*" APS March Meeting 2023, Mar 5-10, 2023, Las Vegas, NV, USA
- (invited) **Kundu, A**. (i)(talk) "Influence of electron-phonon interactions on the electronic properties of materials" & (ii) Hand-on tutorial on i-PI---Qbox coupling for computing electron-phonon renormalization of materials. NOMAD-ECAM Workshop: Modelling Materials at Realistic time Scales via Optimal Exploitation of Exascale Computers and Artificial Intelligence. Jul 25 -29, 2022, Berlin, Germany.
- **Kundu, A.**, Song, Y., Galli, G. "*Revisiting the electronic properties of diamond like amorphous carbon*" APS March Meeting 2022, Mar 14-18, 2022, Chicago, IL, USA
- **Kundu, A.**, Govoni, M., Ceriotti, M., Gygi, F., Galli, G. *"Finite temperature electronic properties of diamond-like carbon materials"* APS March Meeting. Mar 15-19, 2021, Virtual.
- **Kundu, A.**, Govoni, M., Ceriotti, M., Gygi, F., Galli, G. *"Finite temperature electronic properties of diamond and diamondoids"* APS March Meeting. Mar 2-6, 2020, Denver, CO, USA (Cancelled due to COVID-19).
- **Kundu, A**, Sillar, K., Sauer, *"Ab initio prediction of pure and mixture gas adsorption of small molecules in CPO-27-Mg"* Bunsentagung 2016: 115th General Assembly of German Bunsen Society for Physical Chemistry. May 5-7, 2016, Rostock, Germany.
- (invited) **Kundu, A**, Sillar, K., Sauer, J. *"Effects of lateral interactions on adsorption of gas mixtures: an ab initio lattice model study."* Doktorandenseminar (Seminar of Ph.D. students) on Adsorption. Aug 25-26, 2015, Magdeburg, Germany.
- **Kundu, A**, Sillar, K., Sauer, J. *"Ab initio prediction of adsorption isotherms of pure and gas mixtures in CPO-27-Mg"* CECAM Workshop: From the Chemical Bond to the Chemical Plants. Aug 25-29, 2014, Bangalore, India.

Poster Presentations

- **Kundu, A.**, Sillar, K., Sauer, J. *"Ab initio prediction of co-adsorption of gases by GCMC simulations on a lattice of sites."* IMPRS workshop 2018: From Models to Reality. Feb 19 – 23, 2018, Tegernsee, Germany.
- **Kundu, A.**, Sillar, K., Sauer, J., "*Adsorptive separations of small gas molecules using CPO-27-Mg: Insights from ab initio GCMC simulations".* EUROMOF 2017. Oct 29 – Nov 1, 2017, Delft, Netherlands.
- **Kundu, A.**, Sillar, K., Sauer, J. *"Ab initio prediction of co-adsorption of gases by GCMC simulations on a lattice of sites."* WATOC 2017. Aug 27 – Sep 1 , 2017, Munich, Germany .
- **Kundu, A.**, Sillar, K., Sauer, J. *"Ab initio prediction of pure and mixture gas adsorption of small molecules in CPO-27-Mg"* Future of Chemical Physics, J. Chem. Phys. (AIP). Aug 31 – Sep 2, 2016, Oxford, U.K.
- Sillar, K., **Kundu, A.,** Sauer, J. "*Ab initio adsorption thermodynamics of small gas molecules in Mg-MOF-74*" EUROMOF 2015. Oct 11-14, Potsdam, Germany.
- **Kundu, A.**, Piccini, G., Sillar, K., Sauer J. "*Ab initio adsorption thermodynamics of small gas molecules in Mg-MOF-74*", STC 2015. Sep 20 – 24, 2015, Potsdam, Germany.

- **Kundu, A.**, Sillar, K., Sauer, J. *"Ab initio prediction of adsorption isotherm of pure and mixture of gases in Mg-MOF-74"* IMPRS workshop 2015: Micro to Macro. Feb 9 – 13, 2015, Tegernsee, Germany.
- **Kundu, A.**, Sillar, K., Sauer, J. *"Ab initio prediction of adsorption isotherm of pure and mixture of gases in Mg-MOF-74."* STC 2014. Sep 14 – 18, 2014, Vienna, Austria.
- Sillar, K., **Kundu, A.,** Sauer, J. *"Pure gas and mixture adsorption of CO_2 and CH_4 in CPO-27-Mg"* International MOF Symposium 2013, Sep 16 – 17, 2013, Dresden, Germany.

Workshops / Summer schools attended

- MICCoM workshop and Hands-on Tutorials 2022, Oct 13-14, Argonne National Laboratory, Lemont, Illinois, USA.
- European Summer School in Quantum Chemistry (ESQC) 2015, Sep 6 – 19, 2015, Sicily, Italy.
- CECAM Summer School on "Computational modelling for catalysis". Sep 1 – 5, 2014, Bangalore, India.
- International workshop on molecular modelling and simulation: natural science meets engineering, Mar 11 – 12, 2013, Frankfurt/Main, Germany.

PROFESSIONAL SERVICES

Reviewer: Reviewed 15+ manuscripts for journals: *JACS, PNAS, NPJ Comput. Mat. Sci., Commun. Phys., J. Phys. Chem., Phys. Chem. Chem. Phys., Struc. Chem., Crystals, Molecules,* and for *the Czeck Science Foundation (GACR).*

Guest Editor: Served as a guest associate editor in *Frontiers in Catalysis.*

Membership: American Physical Society (2019 – Present), International Max Planck Research School (IMPRS) at Max Planck Society (2012-2018).

Conference Organizer: Organized two triennial IMPRS workshop: (i) From micro to macro, 2015 and (ii) From models to reality, 2018

REFERENCES

1. Prof. Joachim Sauer
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