

## Arpan Kundu, PhD

Staff Scientist, University of Chicago, Pritzker School of Molecular Engineering,  
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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, 1<sup>st</sup> 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 (1<sup>st</sup> class with distinction, Marks 77.7%, 6<sup>th</sup> 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<sup>0</sup> and Au<sup>0</sup> 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”, *J. Phys. Chem. Lett.* **2024**, *15*, 6818.
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](https://arxiv.org/abs/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.**<sup>†</sup>, Sillar<sup>†</sup>, 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<sub>2</sub> 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 1<sup>st</sup> rank in “National Eligibility Test (NET)” examination conducted by CSIR, Govt. of India. Dec 2010
- All India 11<sup>th</sup> 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
- Mentored an undergraduate researcher

December 2022 - Present

June 2020 – Oct 2021

### Humboldt-Universität zu Berlin

Berlin, Germany

- Taught physical Chemistry 2: a practical course for master's students.
- Taught Molecular Modelling (MoMo): a practical course for bachelor's students.
- Supervised a visiting master's student researcher.

Summer 2015, summer 2016

Summer 2013

Summer 2013

## CONFERENCES/WORKSHOPS

### Invited and contributed talks

- **Kundu, A.**, Galli, G. "Quantum vibronic effects on the electronic properties of solid state spin defects" APS March Meeting 2024, Mar 3-8, 2023, Minneapolis, MN, USA.
- **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, J. "Ab initio prediction of pure and mixture gas adsorption of small molecules in CPO-27-Mg" [Bunsentagung 2016: 115<sup>th</sup> 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<sub>2</sub> and CH<sub>4</sub> 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 *Czech 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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Unter den Linden 6. 10117 Berlin.  
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##### 2. Prof. Giulia Galli

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##### 3. Prof. François Gygi

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##### 4. Dr. Michele Ceriotti

Associate Professor,  
École polytechnique fédérale de Lausanne (EPFL),  
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##### 5. Dr. Marco Govoni

Assistant Professor,  
Department of Physics, Computer Science,  
Mathematics.  
University of Modena and Reggio Emilia.  
Via Campi 213/A, Modena, 41125, Italy.  
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##### 6. Dr. GiovanniMaria Piccini

Associate Professor,  
Theoretical & Computational Chemistry, Department of  
Chemical & Geological Sciences,  
University of Modena and Reggio Emilia,  
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