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June 4, 2019

SUBJECT: Application for the post of Post Doctoral Fellow

Dear Sir

I am writing this letter in response to your advertisement on an available post doctoral position in your group.

I have submitted my Ph.D. thesis titled *'Electronic structure and magnetic properties of graphene derivatives and graphene-based composite structures'* carried out under my doctoral advisor Prof. Tanusri Saha-Dasgupta at S.N. Bose National Centre for Basic Sciences, Kolkata, India and am currently awaiting my defence subject to the procedural policy of my parent university, which I expect to be scheduled in Fall.

I have experience with computational materials science in context of using *ab-initio* methods such as density functional theory to investigate various properties (structural, electronic, magnetic, thermodynamic) of different material systems from 0-D nanoparticles/nanoflakes to 2-D materials such as graphene and mxene to 3-D materials such as perovskite materials.

The primary focus of my disseration was to employ computational methods based on density functional theory as well as model Hamiltonian to study different graphene-based systems, *viz adatoms on bilayer graphene, graphene nanoflakes and graphene/stronitum titanate heterostructures*, with the aim of understand the formation of magnetic moments within these systems and, crucially, the tunability of the magnetic and electronic properties when subjected to external perturbations such as external electric field, effect of substrate and chemical modifications.

Further, as part of joint collaborative projects, I have also employed ab-initio methods to investigate the effect of phonon mode softening on the elastic properties of pure and doped Ti_2C *Mxenes*, the role played by geometry in understanding experimentally observed empirical trend found in *metal nanoparticles* and thermodynamic stability analysis in order to estimate growth conditions for the computationally predicted new *Rhodium (Rh)-based double perovskite structures*.

During the duration of my Ph. D. I have published 8 papers in peer-reviewed journals including 3 papers in *ACS Nano* and *Physical Review B* as first author.

The full list of my publications is provided with Curriculum Vitae(which includes a List of Referees) is enclosed along with this Cover Letter.

I kindly request you to consider my application for the post doctoral position in your group.

Thanking You
Ms. Dhani Nafday

CURRICULUM VITAE

Ms. DHANI NAFDAY

Date of Birth: 24^{th} November, 1982

Gender: Female
Citizenship: Indian

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Education

RA-Bridge Fellowship	Indian Association for the Cultivation of Science, India (Oct 2018 - current)
Ph.D.	Physics, S.N.Bose National Center for Basic Sciences, India (2012-2018) Doctoral Advisor: Prof. Tanusri Saha-Dasgupta. Thesis Title: *Electronic structure and magnetic properties of graphene derivatives and graphene-based composite structures* (*Thesis submitted*)
M.Sc.	Physics, Savitribai Phule Pune University, India (2006).
B.Sc.	Mathematics, Fergusson College, Savitribai Phule Pune University, India (2003).

Technical Skills

- Density functional theory simulation packages: VASP, Quantum Espresso, Wien2K
- Operating Systems: Linux, Windows
- Programming: Fortran 77 & 90, C, Linux Shell Scripting, awk, sed
- Applications: LaTeX, Microsoft Office, Gnuplot, Xmgrace, Gimp

Publications

1. A reduction in particle size generally causes body-centered-cubic metals to expand and face-centered-cubic-metals to contract - Dhani Nafday, Subhrangshu Sarkar, Pushan Ayyub and Tanusri Saha-Dasgupta, *ACS Nano* **12(7)**, 7246 (2018)
2. Magnetism of an adatom on bilayer graphene and its control: A first-principles perspective - Dhani Nafday and Tanusri Saha-Dasgupta, *Phys. Rev. B* **88**, 205422 (2013)
3. Controlling adatom magnetism on bilayer graphene by external field - Dhani Nafday, Mukul Kabir and Tansuri Saha-Dasgupta, *Phys. Rev. B* **93**, 045433 (2016)
4. Exact diagonalization study in nanographene: Modulation of charge and spin, magnetic phase diagram, and thermodynamics - Sajeev Chacko, Dhani Nafday, Dilip Kanhere and Tanusri Saha-Dasgupta, *Phys. Rev. B* **90**, 155433 (2014)
5. Out-of-plane dipoles and anti-hysteresis at the interface of graphene-strontium titanate hybrid transistor - Anindita Sahoo, Dhani Nafday, Tathagata Paul, Roald Ruiter, Arunesh Roy, Maxim Mostovoy, Tamalika Banerjee, Tansuri Saha-Dasgupta and Arindam Ghosh, *npj 2D Materials and Applications* **2(9)**, 1 (2018)

6. Search for new magnetic materials : DFT predictions on Rh based double perovskites - Anita Halder, Dhani Nafday, Prabuddha Sanyal and Tansuri Saha-Dasgupta, *npj Quantum Materials* **3(17)**, 1 (2018)

7. Manipulating the mechanical properties of Ti_2C MXene: Effect of substitutional doping - Poulami Chakraborty, Tilak Das, Dhani Nafday, Lilia Boeri and Tansuri Saha-Dasgupta, *Phys. Rev. B* **95**, 184106 (2017)

8. Properties at the interface of graphene and Ti_2C MXene - Pallabi Paul, Poulami Chakraborty, Tilak Das, Dhani Nafday, and Tansuri Saha-Dasgupta, *Phys. Rev. B* **95**, 184106 (2017)

9. Boronated Holey Graphene - A case of 2D ferromagnetic metal - Dhani Nafday, Puru Jena and Tansuri Saha-Dasgupta, *Submitted Phys. Chem. Chem. Phys* (2019)

10. The Curious Case of $NiRh_2O_4$: A Spin-Orbit Entangled Diamond Lattice Paramagnet - Shreya Das, Dhani Nafday, Tansuri Saha-Dasgupta and Arun Paramekanti *Submitted* (2019)

Academic Visits

- Institute of Theoretical and Computational Physics, Graz University of Technology, Austria (June 2016)
  - Supervisor: Ass. Prof. Lilia Boeri
  - Academic visit under joint Indo-Austrian cooperation project, *"Search for superconductivity and magnetism in Mxene phases"*
    - To study the effect of magnetism on the phonon coupling and thus, the mechanical properties of Ti_2C Mxene - [*Phys. Rev. B* **95**, 184106 (2017)]

Presentations in Conferences and Workshops

- Topic: Tunable Magnetism of adatoms on bilayer graphene : A first-principles perspective. (Oral)

  European Graphene Forum 2016: Applications, Developments and Challenges for Graphene and 2D materials. Paris, France from June 1-3 (2016)

- Topic: Magnetism of an adatom on bilayer graphene and its control: A first-principles perspective.(Poster)

  International Symposium on Clusters, Cluster Assemblies and Nano-scale materials-III. Harish-Chandra Research Institute, Allahabad, India from March 11-14 (2014)

  MASTANI 2014: Summer School on Materials Simulation Theory and Numerics. IISER,Pune, India from (June 30 - July 12 2014)

  Runner's Up, Best Poster Competition

Conferences and Workshops attended

- European Graphene Forum 2016: Applications, Developments and Challenges for Graphene and 2D materials Paris, France (June 2016)
- 8^{th} USPEX workshop Shiv Nadar University, New Delhi, India (January 2015)
- MASTANI 2014: Summer School on Materials Simulation Theory and Numerics. IISER Pune, India (June-July 2014)
- International Symposium on Clusters, Cluster Assemblies and Nano-scale materials-III. HRI Allahabad, India (March 2014)

- IUSSTF WORKSHOP 2014: The Physics and Chemistry of Graphene and Other Single and Bilayer Materials including MoS2 and Phospherene IISc Bangalore, India (Jan-Feb 2010)
- International Workshop on Frontiers in Electronic Structure calculations : Techniques and Applications Savitribai Phule Pune University, India (February 2010)

References

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