SCHOOL OF SCIENCES

Name: Himadri R. Soni
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EDUCATIONAL QUALIFICATIONS

Ph.D. (Condensed Matter Physics), 2014, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar, India jointly with The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy (ICTP-IAEA STEP Fellow).

M.Sc. (Physics), 2009, The Maharaja Sayajirao University of Baroda, Vadodara, India.

B.Sc. (Physics, Mathematics), 2007, The Maharaja Sayajirao University of Baroda, Vadodara, India.

Work Experience

Assistant Professor (07/2018 – till date) School of Science, Indrashil University, Rajpur, Mehsana, India.

Postdoctoral Fellow (01/2018 – 06/2018), Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany.

Postdoctoral Fellow (09/2014 – 12/2017), Chair of Theoretical Chemistry, Friedrich-Alexander University of Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany.

SUBJECTS TAUGHT

- Basic Physics I (CH1 102)
- Basic Physics II (CH1 201)
- Basic Physics III (CH2 101)
- Physics (BIO 1-101)
- BioPhysics (BIO2 - 101)
- Engineering Physics (PHY 101)

RESEARCH AREA

- Computational Material Science
- Surface Chemistry
- Novel Carbon Allotropes
- Functionalization of 2D Materials for Energy Applications
- Raman Spectroscopy

Graphene-like two dimensional (2D) materials have recently gained interest especially due to their unique electronic and optoelectronic properties. Graphene and other 2D materials like hexagonal BN, MoS_2 constitute one of the most active fields of research in materials science, condensed matter physics, and chemistry. We have reported a comprehensive study involving in situ Raman spectroscopy supported by quantum mechanical calculations to exactly monitor the covalent binding to graphene with unprecedented precision. We have also studied the reactivity of graphene towards atomic hydrogen for hydrogen storage application (shown in Figure 1).

At present we are working on 2D materials and their functionalization with applications in the field of energy storage. Basically, we are using 2D material as a catalyst to solve two key societal and scientific problems: (1) in the field of environment i.e. CO oxidation to CO_2 in particular, but in general combustion of carbonaceous particulates from engine exhaust gases at room temperature and with high efficiency; and (2) in the field of energy i.e. CO reduction via hydrogenation. The determination of the structure which is required as a basis for understanding many of its properties, in general, a hard task, either by the experimental techniques or by using sophisticated total energy calculations. These calculations will provide fundamental information in relation to element selection, and will also allow us to determine the electronic structure of these systems. This will include the electronic band structure, corresponding density of states, and bonding configurations. Density-functional theory 'DFT' permits calculation of the total energy of solids without any parameterization to experimental data.

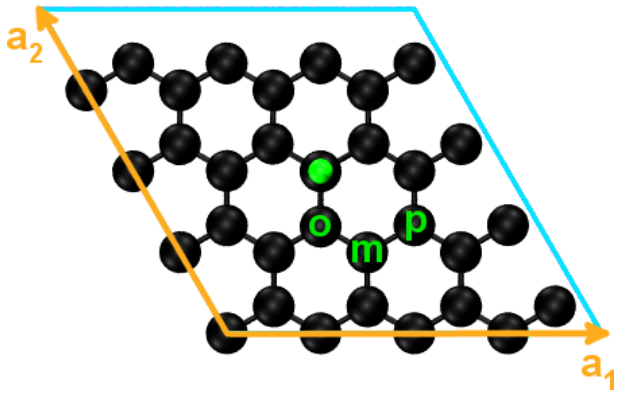

Figure 1: Ortho (o), meta (m), and para (p) functionalization patterns shown for a second hydrogenation with respect to a first hydrogen atom at the position marked by a green circle in a hexagonal (4x4) unit cell (cyan, orange unit cell vectors a_1 and a_2) (Soni et. al., Journal of Physical Chemistry C (2018)).

PROJECTS
NA
Title:
Amount:
Role: Principal Investigator/Co-Principal Investigator
Agency: Full name
Duration: Start and end date

CORE GROUP
Name:
Date of joining:
Topic:

HONOR/AWARD/Fellowship

- Poster award in 1st European Conference on Chemistry of Two-Dimensional Materials (Chem2DMat) at Strasbourg, France (2017).

- ICTP-IAEA STEP fellowship for PhD programme from 2013-2015 at The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

MEMBERSHIP

- **Member –** European Physical Society

PUBLICATIONS

JOURNALS

- Gupta R., Maisel S., Rost F., Weckbecker D., Fleischmann M., **Soni H.**, Sharma S., Görling A. and Shallcros Ms S. **(2019)**. Deformation induced pseudo-magnetic fields in complex carbon architectures. **Physical Review B 100**: 085135: **(IF: 3.836)**.

- Späth F., **Soni H.R.**, Steinhauer J., Düll F., Bauer U., Bachmann P., Hieringer W., Görling A., Steinrück H.P., and Papp C. **(2019).** *Oxygen Functionalization of hexagonal Boron Nitride on Ni(111)*. ***Chemistry - A European Journal*** **25**: 8884-8893: **(IF: 5.160).**

- **Soni H.R.*** and Fyta M **(2018)**. Two-Dimensional Metallic/Semiconducting MoS2 Heterostructure Under Biaxial Strain. **ACS Applied Nano Materials 1(10)**: 5562–5570.

- **Soni H.R.***, Gebhardt J. and Görling A **(2018)**. The Reactivity of Substrate-Supported Graphene: A Case Study of Hydrogenation. **The Journal of Physical Chemistry C 122.5**: 2761–2772: (**IF: 4.484**).

- Astik N. M., **Soni H.**, Jha P.K. and Sathe V. **(2018)**. Influence of Fe Substitution on Structure and Raman Spectra of $La_{0.67}Sr_{0.33}MnO_3$: Experimental and Density Functional Studies. **Physica B 541**: 103: **(IF: 1.453).**

- Keller N., Calik M., Sharapa D., **Soni H.**, Zehetmaier P., Rager S., Auras F., Jakowetz A. C., Görling A., Clark T., and Bein T. **(2018)**. Enforcing Extended J-Aggregate Stacking in Covalent Organic Frameworks. **Journal of American Chemical Society 140 (48)**: 16544–16552: **(IF: 14.357)**.

- Yang Z., Sander T., Schaub T.A., Gebhardt J., Schönamsgruber J., Meinhardt U., **Soni H.**, Ammon M., Görling A., Kivala M., and Maier S. **(2018).** Two-dimensional delocalized states in organometallicacetylide networks on Ag(111). ***Nanoscale* 10**: 3769: **(IF: 7.233)**.

- Prenzel D., Sander T., Gebhardt J., **Soni H.**, Hampel F., Maier S., Görling A., and Tykwinski R.R. **(2017).** *Triethynylmethanol Derivatives: Stable Acetylenic Building Blocks for Surface Chemistry*. ***Chemistry - A European Journal* 23**: 1846-1852: **(IF: 5.160)**.

- Vecera P., Chacón-Torres J.C., Pichler T., Reich S., **Soni H.R.**, Görling A., Edelthalhammer K., Peterlik H., Hauke F., and Hirsch A. **(2017).** Precise Determination of Graphene Functionalisation by in situ Raman Spectroscopy. ***Nature Communications* 8**: 15192: **(IF: 12.353)**.
- Mir S.H., Chakraborty S., Jha P.C., Wärnå J., **Soni H.**, Jha P.K., and Ahuja R. **(2016)**. Two-dimensional Boron: Lightest Catalyst for Hydrogen and Oxygen Evolution Reaction. ***Applied Physics Letters* 109**: 053903: **(IF: 3.495).**

- **Soni H.R.*** and Jha P.K. **(2015)**. Ab-initio study of dynamical properties of two dimensional MoS_2 under strain. **AIP Advances 5**: 107103: **(IF: 1.653)**.

- **Soni H.R.** and Jha P.K. **(2014).** Vibrational and Elastic Properties of 2D Carbon Allotropes: A First Principles Study. **Solid State Communications 189**: 58: **(IF: 1.458)**.

- Gupta S.K., Gupta S.D., **Soni H.R.**, Mankad V., and Jha P.K. **(2014).** A first-principles studies of the superconductivity and vibrational properties of transition-metal nitrides TMN (TM= Ti, V, and Cr). **Materials Chemistry and Physics 143.2**: 503–513: **(IF: 2.084).**

- Jha P.K. and **Soni H.R. (2014).** Strain Induced Modification in Phonon Dispersion Curves of Monolayer Boron Pnictides: A First Principles Study. **Journal of Applied Physics 115**: 023509: **(IF: 2.176).**

- **Soni H.R.** and Jha P.K. **(2013).** A first principles study of thermal properties of Yb-pnictides (YbX, X = N, P, and As) compounds. **Advanced Materials Research 665**: 353–358.

- Gupta S.K., **Soni H.R.**, and Jha P.K. **(2013)**. Electronic and phonon bandstructures of pristine few layer and metal-doped graphene using first principles calculations. **AIP Advances 3**: 032117: **(IF: 1.653).**

- **Soni H.R.**, Mankad V., Gupta S.D., Gupta S.K. and Jha P.K. **(2012).** An abinitio study of ground state, electronic and thermodynamical properties of GaP and Ga_2P. **Journal of Thermal Analysis and Calorimetry 107**: 39–44: **(IF: 2.042)**.

- **Soni H.R.**, Mankad V., Gupta S.K. and Jha P.K. **(2012).** Lattice dynamics and magnetism in FeN and CoN: First principles calculation. **Journal of Alloys and Compounds 522**: 106–113: **(IF: 3.779).**

- Mankad V., Gupta S.K., **Soni H.R.**, and Jha P.K. **(2012).** Density functional theoretical study of lattice specific heat and thermal properties of Magnesium Nitride. **Journal of Thermal Analysis and Calorimetry 107**: 45–48: **(IF: 2.042)**.

- **Soni H.R.**, Gupta S.D., Gupta S.K. and Jha P.K. **(2011).** Density functional theoretical study of the structural, electronic and lattice dynamical properties of Platinum pernitride. **Physica B 406**: 2143–2147: **(IF: 1.453)**.

- **Soni H.R.**, Gupta S.K. and Jha P.K. **(2011).** Abinitio total energy calculation of the dynamical stability of noble metal carbides. **Physica B 406**: 3556: **(IF: 1.453)**.

- **Soni H.R.**, Gupta S.K., Talati M. and Jha P.K. **(2011)**. Ground state and lattice dynamical study of ionic conductors CaF2 , SrF2 and BaF2 using density functional theory. **Journal of Physics and Chemistry of Solids 72**: 934–939: **(IF: 2.048)**.

- Mankad V., **Soni H.R.**, Gupta S.K., and Jha P.K. **(2011).** First Principles Lattice Dynamical Calculation of Semiboride Be2B and its Ternary Alloys XBeB (X=Na, Mg, Al). **Physica B 406**: 3599: **(IF: 1.453).**

BOOKS

- **NA**

BOOK CHAPTERS

- Pillai, S. B., **Soni H. R.,** and Jha P. K. **(2019)** Strain induced changes in Vibrational Properties of Arsenene and Antimonene monolayer, Advances in Spectroscopy: Molecules to Materials, ISSN: 0930-8989, In Press.

CONFERENCES (Selected)

- **Soni, H.,** Gebhardt, J., Yang, Z., Sander, T., Schaub, T.A., Schönamsgruber, J., Meinhardt, U., Ammon, M., Kivala, M., Maier, S., Görling, A, **(2017)** Electronic Properties of Organometallic Graphyne Networks on Ag(111).: 18th International Workshop on Computational Physics, Materials Science: Total Energy, and Force Methods, Trieste, Italy.

- Vecera, P., Chacón-Torres, J. C., Pichler, T., Reich, S., **Soni**, **H. R.,** Görling, A., Edelthalhammer, K., Peterlik, H., Hauke, F., Hirsch, A, **(2017),** Graphene Functionalization by in-situ Raman Spectroscopy, 1st European Conference on Chemistry of Two-Dimensional Materials (Chem2DMat), Strasbourg, France.

- **Soni, H.R.,** Gebhardt, J., Görling, A, **(2016),** Reactivity of Graphene Investigated by Density-Functional Theory, Annual March Meeting of American Physical Society, Baltimore, USA.

- **Soni, H.R.**, Gebhardt, J., Görling, A, **(2015),** Reactivity of Graphene, Symposium on Theoretical Chemistry, Potsdam, Germany.

- **Soni, H.R.,** Jha, P.K., **(2015),** A theoretical analysis of the role of defects and doping in hexagonal boron nitride sheets, 17th International Workshop on Computational Physics, Materials Science: Total Energy, and Force Methods, ICTP, Trieste, Italy.

- **Soni, H.R.,** Jha, P.K., **(2014)**, Strain Induced Vibrational Properties of Monolayer Boron Pnictides, Workshop on Material Challenges in Devices for Fuel Solar Production, ICTP, Trieste, Italy.

- **Soni, H.R.,** Jha, P.K., **(2013),** Electronic and Phonon Engineering of Graphene, National Conference on New Trends in Physics and Material Science, C.S.A. Govt. P.G. College Sehore, Barkatullah University, Bhopal, India.

- **Soni, H.R.,** Gupta, S.K., Jha, P.K., **(2012)**, Electronic and Vibrational Properties of Twisted Graphene, ATHENA-2012, SNBNCBS, Kolkata, India.

- **Soni, H.R.,** Gupta, S.K., Jha, P.K., **(2012)**, Electronic Properties of Twisted Graphene, Methods in Molecular Simulation Summer School 2012, Cardiff University, Cardiff, UK.

WORKSHOP/TRAINING (Selected)

- 12 – 16 March, **2019** (5 days), Inspiring Engineers Through Innovation, Creative Models and Machines, IIT Gandhinagar, India.

- 22 – 31 July, **2012** (10 days), Methods in Molecular Simulation Summer School 2012. Cardiff University, Cardiff, UK.

- 1 – 30 June, **2012** (30 days), Short Term Visit Programme. Condensed Matter and Statistical Physics Division, ICTP, Trieste, Italy.

- 3 – 13 November, **2010** (11 days) School on Understanding Molecular Simulations Theory and Applications. IIT-Kanpur, Kanpur, India.

- May – June **2008** (2 months), Visiting Student Research Programme. TIFR, Mumbai, India.

PATENTS/ TECHNOLOGY TRANSFER

- NA

OTHER INFORMATIOS

- **Reviewer of peer reviewed journals:**
  Solid State Communications, Journal of Alloys and Compounds, Physica B, Carbon, Chemical Physics Letters, Computational Materials Science, Journal of Semiconductors, Journal of Applied Physics, Optical Materials.