Academic Report (2020-21)

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Research Summary:

In this period we focussed on two major themes: materials for alternative energy; fundamental understanding of magnetic materials.

We explored a class of ternary transition metal tri-chalcogenide compounds for their efficiency as electrocatalysts in hydrogen evolution reaction. We identified 10 new stable compounds with this property. We also developed new insights into how catalytic efficiency of some of the known compounds can be increased further.

We collaborated with the experimental group of Dr. T. N. Narayanan of TIFR, Hyderabad to develop microscopic understanding of how cobalt decorated nitrogenated graphitic carbon spheres (Co-NGC) work as good bi-functional catalyst for oxygen evolution and oxygen reduction reactions (OER/ORR). This property makes Co-NGC a promising cathode material in rechargeable Zn-air batteries. We also developed a theoretical understanding of how a mixed (KOH+LiOH) electrolyte enhances cyclability of rechargeable Zn-air batteries.

In fundamental studies, we developed new theoretical understanding into magnetic properties of Co_2C nano-particles in collaboration with the experimental group of Prof. S. Banerjee at IIT-Kanpur, who had found nano-particles of this material to show complex magnetic behavior including large magnetic anisotropy energy. We also developed new insights into electronic and magnetic properties of the tri-chalcogenide compounds.

Publications:

1. K. Alam, N. Seriani and P. Sen, *Catalytic properties of α-MnO_2 for Li-air battery cathodes: a density functional investigation,* Phys. Chem. Chem. Phys. **22**, 9233, (2020).

2. P. Sen and R. Chouhan, *Electronic structure of MPX_3 tri-chalcogenide monolayers in density functional theory: A case study with four compounds (M=Mn, Fe; X=S, Se),* Elec. Str. **2**, 025003, (2020).

3. P. Sen, K. Alam, T. Das, R. Banerjee and S. Chakraborty, *Combinatorial design and computational screening of 2D transition metal tri-chalcogenide monolayers: Toward efficient catalysts for hydrogen evolution reaction,* J Phys. Chem. Lett. **11**, 3192, (2020).

4. P. Thakur, M. Yeddala, K. Alam, S. Pal, P. Sen, and T. N. Narayanan, *Cobalt Nanoparticles Dispersed Nitrogen-Doped Graphitic Carbon Nanospheres-Based Rechargable High Performance Zinc-Air Batteries,* ACS Appl. Energy Mater. **3**, 7813, (2020).

Preprints:

1. K. Alam, T. Das, S. Chakraborty and P. Sen, *Finding the catalytically active sites on the layered tri-chalcogenide compounds $CoPS_3$ and $NiPS_3$ for hydrogen evolution reaction,* (submitted).

2. T. Das, K. Alam, S. Chakraborty and P. Sen, *Probing active sites on $MnPSe_3$ and $FePSe_3$ tri-chalcogenides as a design strategy for better hydrogen evolution reaction catalysts*, (submitted).

3. P. Thakur, K. Alam, P. Sen and T. N. Narayanan, *Extending the Cyclability of Alkaline Zinc-Air Batteries: Synergistic Roles of Li^+ and K^+ Ions in Electrodics*, (submitted).

4. N. Roy, M. A. Ali, A. Sen, P. Sen and S. Banerjee, *Evidence of Exchange Bias effect in pure Co_2C nanoparticles*, arxiv.org/abs/2005.04904 (submitted).

Conference/Workshops Attended:

1. *Webinar Series on Materials Simulation: A Virtual Guided Tour*, India, May, 2020.

2. *Conference on Quantum Condensed Matter Physics (QMAT-2020)*, India, July, 2020.

Invited Lectures/Seminars:

1. *Layered ternary tri-chalcogenides and Co-based clusters: Energy applications and new insights*, Webinar Series on Materials Simulation: A Virtual Guided Tour, IIT, Delhi, online, May, 2020.

2. *Screening layered ternary transition metal tri-chalcogenides as electrocatalysts*, Conference on Quantum Condensed Matter Physics (QMAT-2020), S. N. Bose National Centre for Basic Sciences, Kolkata, online, July, 2020.

Other Activities:

1. Participated in the Vaibhav Summit in the Computational Materials Science horizontal, October, 2020.

2. Editorial Board Member of *Physica Scripta*.

3. Convener Cluster Committee, member Colloquium Committee, Physics Academic Committee.

4. Dean Academic since March 2020.

5. Teaching courses: Condensed Matter Physics 1, Spectroscopic Methods.