SINP Newsletter

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Mechanism of Versatile Catalytic Activities of Quaternary CuZnFeS Nanocrystals Designed by a Rapid Synthesis Route

Amit Dalui[1], Umamahesh Thupakula[1], Ali Hossain Khan[1], Tanmay Ghosh[2], Biswarup Satpati[2], and Somobrata Acharya[1]

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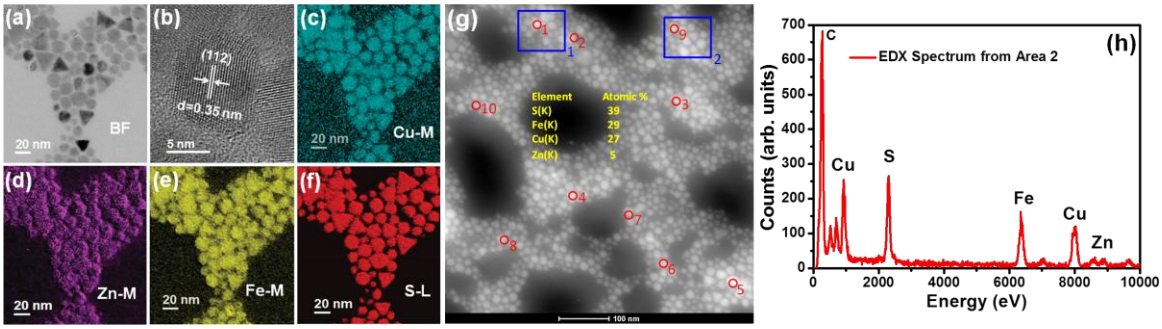
Quaternary alloyed nanocrystals (NCs) composed of earth abundant, environment friendly elements are of interest for energy-harvesting applications. These complex NCs are useful as catalysts for the degradation of multiple refractory organic pollutants as well as nitro-organic reduction at a rapid rate. Here, a remarkably fast (~30 s) and facile synthesis of crystalline quaternary chalcopyrite copper-zinc-ironsulfide (CZIS) NCs is reported. These NCs show excellent catalytic properties by degrading a number of refractory organic dyes and converting nitro-compounds at a rapid rate. The valence and conduction band information of the newly designed NCs are extracted using scanning tunneling spectroscopy and ultraviolet photoelectron spectroscopy, which reveal energy levels suitable for performing redox chemistry by generating reactive radicals establishing NCs as effi cient catalyst with multiple uses. Rapid synthesis of high quality phase-controlled CZIS NCs with robust catalytic activities could be useful for organic waste treatment.

Figure. a) TEM image and b) high-resolution-TEM image of CZIS NCs. c–f) Chemical maps of the constituent elements measured using an EFTEM technique, showing copper, zinc, iron, and sulfur. g) STEM-HAADF image of CZIS NCs. Inset: EDX data showing quantitative percentage of the elements present in the CZIS NCs. h) EDX spectrum of CZIS NCs revealing the presence of Cu, Zn, Fe, and S. The EDX was collected from the blue square area marked in panel (g).



Full Journal Reference: ***small*** *2014, DOI: 10.1002/smll.201402837*

No of authors from outside SINP: 4

Oxidative Tearing of Graphene Sheets: Insights into the Probable Situations by Computational and Experimental Studies

Angana Ray, Koushik Bagani, Sangam Banerjee and Dhananjay Bhattacharyya

Functionalization of graphene is a big challenge to make these nano-materials biologically active. Oxydation of graphene appeared as a possible solution. We, however, found oxydation of graphene can lead to tearing it into smaller pieces. Our theory suggested that the smaller graphene molecules would have n^2 number of carbon atoms, somewhat quantized, which needs to be verified through experiments.

Abstract:
Nanometer size graphene sheet has become a subject of interest both for technological as well as medical applications. In this work, we have focused on the oxidative tearing of nanoscale graphene sheets using *ab initio* density functional theory. We have geometry optimized several model systems depicting all possible graphene oxide sheets containing either a single or multiple oxygen atoms. We have found that a single oxygen atom prefers to bind to two carbon atoms of the cis-edge by forming an epoxy linkage. Such epoxidation also induces a large curvature into the graphene sheet by breaking the involved C− C bond. This initial epoxidation also favors formation of similar epoxy-linkages at nearby sites in a cooperative manner during the oxidation of a nascent graphene sheet. Such bond breaking, however, is not observed when we try similar epoxidation at the trans-edge. A series of epoxidation starting from the cis-edge thus can cause tearing of the graphene oxide sheet leading to formation of smaller size graphene sheets containing exposed functionalized trans-edges. Because of symmetry in a graphene sheet, we can expect to obtain a smaller functionalized graphene sheet of triangular shape having predominantly trans-edges (cis edges may appear at the corners) during the oxidation process. Our subsequent experiment of magnetic hysteresis compliments the theoretical finding of the tearing pattern.

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J. Phys. Chem. C (2014) DOI: 10.1021/jp511001f

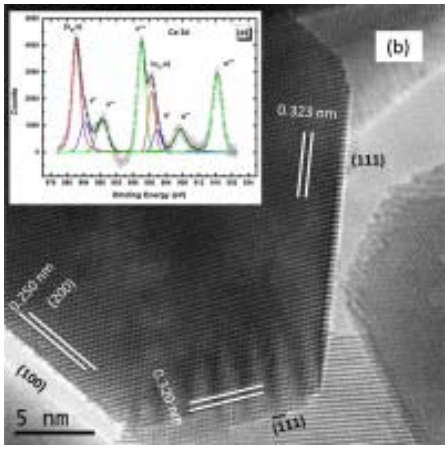
All the authors are SINP members

Research

TEM and XPS Studies on the Faceted Nanocrystals of $Ce_{0.8}Zr_{0.2}O_2$

Manabendra Mukherjee

Faceted nanocrystals of $Ce_{0.8}Zr_{0.2}O_2$ synthesised by co-precipitation method were characterised by X-ray diffraction, high-resolution transmission electron microscopy, Thermogravimetry - Differential Scanning Calorimetry and X-ray photoelectron spectroscopy techniques. The nanocrystals were highly faceted and exhibited a cubic phase. X-ray photoelectron spectroscopy analyses confirmed the presence of vacancy related defects and revealed the presence of~ 22% of Ce^{3+} in the nanopowders. High-resolution transmission electron microscopy results confirmed that the nanocrystal sizes are around 31±5 nm and the obtained hexagonal cross-section shape is bound by hexagonal {111} and square {100} facets. The shape-controlled nanocrystals were synthesised without using any surfactants or complexing agents and retained their morphology beyond 800 ºC. This is a simple and easy method for producing shape-controlled $Ce_{0.8}Zr_{0.2}O_2$ nanoparticles which can be used for catalytic conversion and other related advanced technological areas.



Ref: Materials Characterization 100 (2015) 31–35

Authors from outside SINP: 4

Nonlinear wave collapse, shock and breather formation in an electron magnetohydrodynamic plasma

Nikhil Chakrabarti [1]

Low-frequency nonlinear wave dynamics is investigated in a two-dimensional inhomogeneous electron magnetohydrodynamic (EMHD) plasma in the presence of electron viscosity. In the long-wavelength limit, the dynamics of the wave is found to be governed by a novel nonlinear equation. The result of the moving-frame nonlinear analysis is noteworthy, which shows that this nonlinear equation does have a breather solution and electron viscosity is responsible for the breather. A breather is a nonlinear wave in which energy accumulates in a localized and oscillatory manner. Analytical solution and time-dependent numerical simulation of this novel equation reveal the collapse of a soliton (localized pulse) into a weak noise shelf and formation of shocklike structures.

Ref. PHYSICAL REVIEW E 90, 063111 (2014)
http://dx.doi.org/10.1103/PhysRevE.90.063111

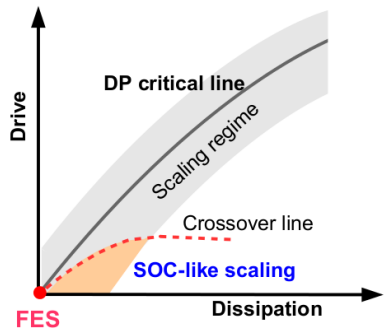
[1]Author outside SINP: Samiran Ghosh, University of Calcutta (applied Math)

Self organised criticality is connected to Percolation

Urna Basu and P. K. Mohanty

December 24, 2014

Self organized critical (SOC) systems are those which have potential to become catastrophically unstable to small perturbations. A socio-economic system may become catastrophically unstable while trying to achieve an optimal state or a pile of snow flakes may produce catastrophic avalanches. Or as pointed out recently, the neuronal activity in the human brain too follows the principles of self-organization. Large events are quite typical in these systems, which are charaterized by scale-free distributions of size or duration of avalanches they produce. One important question, which remained unanswered is, 'are there universality' in these self critical states? Can we classify the self critical state similar to an ordinary system at a critical point ?



The most generic universality class of self-organized systems, usually modeled by sandpile models, is believed to be Manna-universality class (MC), with critical exponents different from Directed Percolation (DP), a similar model at ordinary critical point. This has been a puzzle for a long time, and is still being debated. The only way to ascertain this is to estimate the critical estimates of both models and compare, which is computationally expenssive, as these nonequilibrium systems are quite complex and bring in undesirable transient effectes.

In this work we provide a strong argument, and show both in one and higher dimensions, that the ordinary critical behaviour (DP) can be extended to slow-drive dissipation regime, where the scaling regime splits and the DP critical behaviour crosses over to a new state with emerging SOC-like feature. We show that the critical exponets in this regime, which includes the usual SOC, are only DP-exponents, but rescaled.

Journal Ref.: *SOC in stochastic sandpiles: connection to DP,*
U. Basu and P. K. Mohanty, EPL **108**, 60002 (2014).

Authors from SINP : One .

Effect of pressure on the magnetic and superconducting transitions of $GdFe_{1-x}Co_xAsO$ (x =0, 0.1, 1) compounds

D. Bhoi, A. Midya and P. Mandal

We have investigated the effect of applied pressure (P) on the magnetic and superconducting transitions of $GdFe_{1-x}Co_xAsO$ (x=0, 0.1, 1) compounds by measuring the temperature dependence of resistivity. At ambient pressure, GdFeAsO undergoes a spin-density-wave transition at T_N =128.2 K associated with the 3d electrons of Fe. Under external pressure, T_N decreases from 128.2 K at 0 GPa to 114.5 K at 2.5 GPa at the rate dT_N/dP=6 K/GPa. Unlike GdFeAsO, the isostructural GdCoAsO exhibits a ferrimagnetic ordering of the Co moments at $T_{FM}^{Co} \sim 76$ K which decreases from 76 K to 71 K as pressure increases from 0 to 2.5 GPa. For the $GdFe_{0.9}Co_{0.1}AsO$ sample, the superconducting onset temperature T_c^{on} decreases monotonically from 19 to 17.1 K, and the temperature T_c^{zero} at which the resistivity disappears decreases from 16.7 to 10.5 K as pressure increases from 0 to 2.9 GPa. For all the three samples, both the value of resistivity and the strength of electron-electron correlation decrease monotonically with increasing pressure.

Journal Reference: Supercond. Sci. Technol. 28, 015009 (2015)

No. of authors outside SINP is 2

Giant magnetocaloric effect in ferromagnetic superconductor $RuSr_2GdCu_2O_8$

A. Midya and P. Mandal
Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Calcutta 700 064, India
(Dated: December 18, 2014)

We have investigated the magnetic and magnetocaloric properties of ferromagnetic superconductor $Ru(Sr_{1-x}La_x)_2GdCu_2O_8$ (x=0-0.10) by magnetization and heat capacity measurements. $RuSr_2GdCu_2O_8$ shows onset of superconductivity at around 46 K which coexists with the weak ferromagnetic ordering of the RuO_2 moments and the antiferromagnetic ordering of the Gd moments. Both superconducting $RuSr_2GdCu_2O_8$ and non-superconducting $Ru(Sr_{0.9}La_{0.1})_2GdCu_2O_8$ compounds exhibit a large magnetic entropy change due to the field-induced metamagnetic transition. The maximum values of entropy change, adiabatic temperature change and refrigerant capacity are $\sim$15.5 J kg^{-1} K^{-1}, $\sim$14 K and $\sim$125 J kg^{-1}, respectively for a field change of 0-7 T for both the compounds. These magnetocaloric parameters also have reasonably good values for a moderate field change (2-3 T), therefore, fulfilling the necessary conditions for refrigeration in the low-temperature region.

Reference: J. Appl. Phys. 116, 223905 (2014)

The following is the thesis work of our student, Mr. Palash Khan. His thesis work in ALICE has led to two Phys. Lett. B publications during 2014. He will be submitting his thesis shortly.

The students and faculties from SINP involved in ALICE Collaboration are:
Palash Khan, Biswarup Paul, Sukalyan Chattopadhyay, Debasish Das, Pradip K. Roy and Tinku Sinha.

Physics Letters B 740 (2015) 105–117

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Physics Letters B

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Production of inclusive $\Upsilon(1S)$ and $\Upsilon(2S)$ in p–Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV

ALICE Collaboration *

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ABSTRACT

We report on the production of inclusive $\Upsilon(1S)$ and $\Upsilon(2S)$ in p–Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV at the LHC. The measurement is performed with the ALICE detector at backward ($-4.46 < y_{cms} < -2.96$) and forward ($2.03 < y_{cms} < 3.53$) rapidity down to zero transverse momentum. The production cross sections of the $\Upsilon(1S)$ and $\Upsilon(2S)$ are presented, as well as the nuclear modification factor and the ratio of the forward to backward yields of $\Upsilon(1S)$. A suppression of the inclusive $\Upsilon(1S)$ yield in p–Pb collisions with respect to the yield from pp collisions scaled by the number of binary nucleon–nucleon collisions is observed at forward rapidity but not at backward rapidity. The results are compared to theoretical model calculations including nuclear shadowing or partonic energy loss effects.

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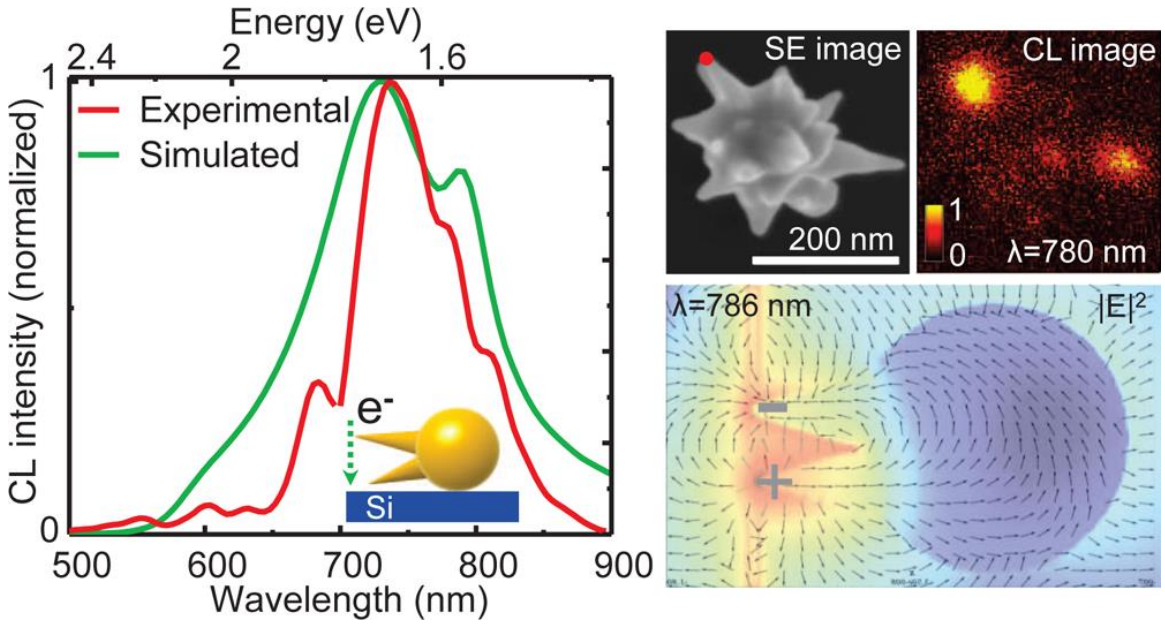
Effect of Intertip Coupling on the Plasmonic Behavior of Individual Multitipped Gold Nanoflower

Achyut Maity, Arpan Maiti, Pabitra Das, Dulal Senapati,

and Tapas Kumar Chini

We report here, the first experimental realization on the selective excitation of two closely lying tips from the same spherical core of a multitipped gold nanoparticle with flower-like morphology. This gives strong multipeaked resonance in the near-infrared region of the far field emission spectra showing a clear signature of tip to tip coupling. The cathodoluminescence (CL) technique in a scanning electron microscope (SEM) combined with finite-difference time-domain (FDTD) simulation has helped us to identify the coupled plasmon modes to be originated from the interaction between two closely spaced tips with a narrow angular separation. Our analysis further estimates a range of angular separation between the tips that triggers the onset of the intertip coupling.



Ref : *ACS Photonics* 2014, 1, 1290-1297

MISCELLANEOUS NEWS/INFO

- International Award in Experiment:

The Hevesy Medal Award Selection Panel 2015 (HMASP-15) has announced that two candidates have been selected to receive the Hevesy Medal Award 2015 (HMA-15). Their names, in alphabetical order, are:

- Professor Dr. Kattesh V. KATTI of the Center for Radiological Research, University of Missouri-Columbia, Columbia, MO, U.S.A.,
- **Professor Dr. Susanta LAHIRI** of the Chemical Sciences Division, Saha Institute of Nuclear Physics, Kolkata, India.

For the first time someone from INDIA will be receiving this award.

The Hevesy Medal Award is the premier international award of excellence honouring outstanding achievements in radioanalytical and nuclear chemistry. The Hevesy Medal was awarded almost annually during the period 1968-86 to nineteen distinguished individuals whose contributions had traced and defined the scope and depth of radioanalysis through the prolific postwar years of the nuclear era. Their achievements included pioneering work on radioactivation analysis methodology and applications, the development of radiochemical separation procedures and analytical schemes, radiotracer applications, analytical developments such as substoichiometric isotopic dilution analysis, automated systems and computerized systems, and widespread fields of application. After an interval of 14 years, the Award was reactivated in 2000.

The International Committee on Activation Analysis of the Modern Trends in Activation Analysis Conferences (ICAA-MTAA) is currently responsible for administration of the award. Announcement issued by: Professor Dr. A. Chatt, Chair, Hevesy Medal Award Selection Panel 2015, President, ICAA/MTAA, Chair, JRNC Board of the Hevesy Award, chatt@dal.ca, 2014 November 30.

Two of our faculty members have been selected as Fellows of the Indian Academy of Sciences, Bengaluru: Profs. **Anjan Kundu** and **Gautam Bhattacharyya** of Theory Division.