



SURNAME, NAME	TITLE
AGBAOYE, Ridwan Olamide	Calculations on optimized structured Poly (3,4-ethylenedioxythiopene) PEDOT
AHMED, Muhammad Hamdy	Absorption enhancedment in hexagonal plasmonic solar cell
ANTIPINA, Liubov Yu	Bilayered semiconductor graphene nanostructures with periodically arranged hexagonal holes as perspective material for photovoltaics
ATAEI, Seyedeh Samaneh	Ab-initio study of oxygen vacancy and hydrogen doping in anatase TiO2
AZIMIGEHRAZ, Seyedjavad	Structural and electronic properties of Li2CoPO4F as Cathode material in Lithium-ion batteries
AZIZI, Khatereh	Molecular dynamics study of gas separation by flexible graphyne-3 sheet





SURNAME, NAME	TITLE
BAG, Saientan	Dramatic changes in DNA conductance with stretching: Structural Polymorphism at a critical extension
BENSLIMANE, Abdelhakim	Thermal effect on the microstructure of Carboxymethyl cellulose: Rheological consideration
CARNEVALI, Virginia	Atomic scale investigation of graphene Moire' structures on NI(100)
CHEN, Lei	Using the fractional-dimensional approach (FDA) to study exciton binding energies in GaAs films on Al _x Ga _{1-x} As substrates
DEBNATH, Saikat	Identifying optimal dye sensitizers for use in solar cells: A density functional theory study
DOMINGUEZ CASTRO, Adrian	Adsorption on a nanoporous organic polymer for clean energy application: A multiscale modeling study using Density Functional Tight Binding Approach





SURNAME, NAME	TITLE
GUEDES-SOBRINHO, Diego	(Meta)stability and dynamics of gold nanoclusters at finite-temperature
LISOVSKI, Oleg	DFT modelling of doped ZnO nanowires with various diameters
LIU WenLiang	Anisotropic interactions and strain-induced topological phase transition in Sb_2Se_3 and Bi_2Se_3
LUKOYANOV, Alexey V.	Accounting for spin-orbit coupling and electronic correlations in calculations of the electronic structure of actinide materials
MARTIN, Henry	An algorithm to calculate the ground state (low-spin) energy and force of multi-centre transition metal (MCTM) complexes
MATERZANINI, Giuliana	Water adsorption at metal surfaces: A first principles study of the $p(\sqrt{3}x\sqrt{3})R30^{\circ}H_{2}O$ bilayer on Ru(0001)





SURNAME, NAME	TITLE
MISRA, Debolina	Theoretical analysis of the physical properties of LaNiO3 and its applications in solid oxide fuel cells and batteries
MISTRY, Aashutosh and MUKHERJEE, Partha P.	Improving discharge performance of Li-air batteries with electrode microstructural modifications
MOHAMED, Fatema Yahya	Nanoclusters on graphene/lr(111): Insights from ab-initio calculations and experiments
MONTAZERI HEDESH, Abbas	Molecular dynamics simulation of hydrogen storage in graphene-like MoS2 nanosheets
MORTAZAVI GHEPCHAGH, Fariba	Granular chain translocation in the horizontally vibrated periodic ratchet channel
OUYANG, Gang	Surface and size effects of nanostructures with negative curvature





SURNAME, NAME	TITLE
PUTUNGAN, Darwin Barayang	A first-principles examination of conducting monolayer 1T'-MX ₂ (M=Mo, W; X=S, Se, Te): Promising catalysts for hydrogen evolution reaction and its enhancement by strain
REN, Ren	Spin-orbital fluctuating dynamics using enhanced Raman shift of magnetic resonance force microscopy in ferromagnetic correlated electronic system perovskite multi-films
SAIMA, Kalsoom	Cytokine interleukin-2 (<i>IL-2</i>) as a prevalent role in the growth, activation and differentiation of T cells.
SARKAR, Utpal	First princple study of graphyne and its derivatives
SEGEV, Elad	Electronic properties of nanocrystalline π -SnS and π -SnSe - a new cubic phase of Tin sulfide and tin selenide
SEIXAS ROCHA, Leandro	Multiferroic two-dimensional materials





SURNAME, NAME	TITLE
SHUKLA, Garima	3-D simulations of slurries for electrochemical energy storage applications
SI, Chen	Half-metallic ferromagnetism and surface functionalization-induced metal-insulator transition in graphene-like two-dimensional Cr ₂ C crystals
SOARES FERREIRA NUNES TEIXEIRA, Sofia Luisa	Geometrical optimization of a thermoelectric device
THANGAVEL, Vigneshwaran	A multiscale model to study the discharge of lithium sulfur batteries
TREJO BANOS, Alejandro	Surface Lithium effects on the structure and electronic properties of porous silicon
TRIVEDI, Ravi Kumar	Study of adsorption and dissociation pathway of H2molecule on MgRh (n=1-10) clusters: A first principle investigation





SURNAME, NAME	TITLE
TSHWANE, David Magolego	Generation of MnO₂nanotubes using computer simulation techniques
TUMURBAATAR, Tsevelmaa	Magnetization reversal of magnetic anisotropy in Li _x FePO ₄
ULMAN, Kanchan Ajit	Passivation of surface states of alpha-Fe ₂ O ₃ (0001) surface by deposition of Ga ₂ O ₃ overlayers: A density functional theory study
VORONTSOV, Alexander	Multiscale approach to simulating the metal vapor condensation
YU, Jing	The simulation of Majorana qubits by Ising chain
ZARBO, Liviu	Influence of electric field on methane adsorption in metal-organic frameworks