List of Publications arising from the thesis

Journal

1. “Complexation behavior of trivalent actinides and lanthanides with 1,10-phenanthroline-2,9-dicarboxylic acid based ligands: Insight from density functional theory.”

2. “Theoretical prediction of icosahedral U@C_{20} and analogous systems with high HOMO-LUMO gap.”


5. “Pu@C_{24}: A new example satisfying 32-electron principle.”

6. “Actinide selectivity of 1,10-phenanthroline-2,9-dicarboxamide and its derivatives: A theoretical prediction followed by experimental validation.”
7. “Complexation of Am$^{3+}$ and Eu$^{3+}$ ions with thiophosphinate ligands involving oxygen and sulphur donors: A density functional investigation.”


**Conferences**

1. “New series of stable actinide and lanthanide encapsulated fullerene systems”


2. “Lanthanide/actinide encapsulated icosahedral C$_{20}$ fullerene system: A density functional prediction”


3. “Different spin states of trivalent Americium and Europium complexes with selective sulphur donor ligands”


4. “Effect of solvent polarity and spin-orbit interaction on the excited states of uranyl Ion”


5. “Trivalent actinide and lanthanide complexes with derivatives of 1,10-phenanthroline-2,9-dicarboxylic acid: A density functional investigation”

Others

1. “Theoretical prediction of XRgCO\(^+\) ions (X = F, Cl and Rg = Ar, Kr, Xe).”

2. “Structure and stability of Zn, Cd, and Hg atom doped golden fullerene (Au\(_{32}\)).”

3. “Theoretical prediction of rare gas containing hydride cations: HRgBF\(^+\) (Rg = He, Ar, Kr, and Xe).”

4. “Theoretical prediction of rare gas inserted hydronium ions: HRgOH\(_2\)^+ ions.”

5. “Significant modulation of CO adsorption behaviour on the various sites of Li doped Au\(_{20}\) cluster.”

7. “Hindered rotation in a Novel 1,2,4-triazinyl phenanthroline (t-phen) ligand leading to improved separation of Am^{3+} and Eu^{3+} vis-á-vis 1,2,4-triazinyl bipyridine (t-bipy): A computational validation of the experimental results.”

8. “Synthesis, characterization, photoluminescence and computational studies of monoorgano - gallium and -indium complexes containing dianionic tridentate ONE (E = O or S) schiff bases.”


10. “Complexation of thorium with pyridine monocarboxylates: a thermodynamic study by experiment and theory.”


12. “Synthesis, structures and DFT calculations of 2-(4,6-dimethyl pyrimidyl)selenolate complexes of Cu(I), Ag(I) and Au(I) and their conversion into metal selenide nano-crystals.”


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