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PUBLICATIONS:

1. V Ashwin, MB Ahamed, SB Elavarasi (2020). Structural, electronic, magnetic and half-metallic properties of cubic perovskites NaBeO₃ and KBeO₃ using PBE-GGA and TB-mBJ approach: A DFT perspective. Applied Physics A 126 (11), 1-11.
2. M Guin, S Khanna, SB Elavarasi, P Sarkar (2020). DFT calculations, Hirshfeld surface analysis and docking studies of 3-anisaldehyde thiosemicarbazone. Journal of Chemical Sciences 132, 81.
3. SB Elavarasi, S Divya, MV Priya, MS Sirajuddeen (2020). NMR, magnetic and electronic investigations of fluorinated nanotubes with different coverage of fluorine. Chemical Physics Letters 742, 137142.
4. M Mohamed Sheik Sirajuddeen, M Sundareswari, I Raja Mohamed, S Begam Elavarasi, Ikram Nabi Lone, Nazir ahmed Teli, S Syed Rahmathulla, Mohammed Shoaib Hussain (2020). A DFT+ U study to report magnetic phase transition, electronic properties and half metallic ferromagnetism in palladium oxide using Hubbard method. Materials Chemistry and Physics 241, 122263.
5. M Mohamed Sheik Sirajuddeen, M Sundareswari, I Raja Mohamed, S Begam Elavarasi, Ikram Un Nabi Lone, Nazir Ahmad Teli, Syed Rahmathulla, Mohammed Shoaib Hussain (2019). Computational Condensed Matter 21, e00425.
6. S Divya, A Kumari, SB Elavarasi (2019). A DFT investigation of the dependence of C13 and F19 CSA parameters on diameter and surface decorated functional groups in F-SWCNTs. Materials Chemistry and Physics 223, 715-722.
7. SB Elavarasi, D Mariam, MU Momeen, J Hu, M Guin (2019). Effect of fluorination on bandgap, first and second order hyperpolarizabilities in lithium substituted adamantane: A time dependent density functional theory. Chemical Physics Letters 715, 310-316.