

# Dr mohamed sheik sirajuddeen

## List of Publications by Year in descending order

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8  
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#	ARTICLE	IF	CITATIONS
1	Structural, electronic, magnetic and half-metallic properties of cubic perovskites NaBeO <sub>3</sub> and KBeO <sub>3</sub> using PBE-GGA and TB-mBJ approach: A DFT perspective. Applied Physics A: Materials Science and Processing, 2020, 126, 1.	2.3	16
2	A density functional calculations on electronic, magnetic, optical, mechanical and half-metallic properties in molybdenum based pnictogens in GGA and GGA+U approach. Materials Chemistry and Physics, 2021, 260, 124159.	4.0	8
3	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, 2020, 241, 122263.	4.0	7
4	Investigation of half-metallic ferromagnetism in hafnium and tantalum doped NiO for spintronic applications: A DFT study. Current Applied Physics, 2019, 19, 357-362.	2.4	4
5	A comparison study of the structural, electronic and magnetic properties in zinc-blende Pt <sub>x</sub> Cr <sub>1-x</sub> P and Rh <sub>x</sub> Cr <sub>1-x</sub> P (x = 0.125, 0.25), and half-Heusler XCrP (X = Pt, Rh): First principles calculations. Materials Chemistry and Physics, 2019, 230, 151-161.	4.0	3
6	Nitrogen induced half metallic ferromagnetism in oxides of calcium and cadmium: A DFT perspective. Materials Chemistry and Physics, 2020, 243, 122336.	4.0	2
7	Electronic and Magnetic properties of nitrogen substituted cubic perovskites of RbNbO <sub>3</sub> and CsNbO <sub>3</sub> using PBE-GGA and TB-mBJ methods. Materials Research Innovations, 0, , 1-12.	2.3	2
8	A DFT investigation of electronic, elastic, and thermal properties of 3d transition metal carbides $\text{TM} \text{C}$ (TM = Sc, Zn). Computational Condensed Matter, 2020, 25, e00500.	2.1	1