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# Electronic Supplementary Information (ESI) Materials:

## Half-metallic double perovskite oxides: recent developments and future perspectives

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**Table S1** The fundamental structural and physical properties, synthesized methods, structural characterized methods and applications of half-metallic double perovskite oxides as well as the device's performance based on such family of materials

| HM DP oxides | Description | | | | Ref. |
|---|---|---|---|---|---|
| Basic fundamental properties | Structure | Goldschmidt's tolerance factor (t) | | Crystal structure | S1 |
| | | $t=\frac{\langle r_A\rangle + r_O}{\sqrt{2}(\frac{<r_{B'}>+<r_{B''}>}{2}+r_O)}$ | $1.05 < t$ | Hexagonal | S2,<br>S3,<br>S4 |
| | | | $1.00 < t < 1.05$ | Cubic | |
| | | | $0.97 < t < 1.00$ | Tetragonal | |
| | | | $t < 0.97$ | Orthorhombic (Pbnm) /monoclinic (P21/n) | |
| | Physical properties | High Curie temperature ($T_C$), magnetization ($M$), magnetoresistance (MR), and high electron polarizability ($P$) | | | S5-S8 |
| Synthesis of HM DP oxides | 0D HM DP oxides | Solid-state reaction (SSR) method combining with high-energy ball milling process | | | S9 |
| | | Molten salt synthesis (MSS) method | | | S10 |
| | | Sol-gel process | | | S11 |
| | | Coprecipitation method | | | S12 |
| | | Combustion method | | | S13 |
| | | Hydrothermal method | | | S14 |
| | 1D HM DP oxides | Hydrothermal method | | | S15 |
| | 2D HM DP oxides | Pulsed laser deposition (PLD) | | | S16 |
| | | Magnetron sputtering | | | S17 |
| | | Chemical solution deposition (CSD) | | | S18 |
| | 3D HM DP oxides | Solid-state reaction (SSR) method<br>Spark plasma sintering method<br>Floating-zone method | | | S19<br>S20<br>S21-S23 |
| Microstructural characterization techniques | X-ray diffraction (XRD)/neutron diffraction (ND) methods | | | | S24 |
| | Scanning/transmission electron microscopy (S/TEM) | | | | S25 |
| | Energy dispersive X-ray spectroscopy (EDS) | | | | S26 |
| | Electron energy loss spectroscopy (EELS) | | | | S27 |
| | X-ray photoelectron spectroscopy (XPS) | | | | S28 |
| | X-ray magnetic circular dichroism (XMCD) | | | | S29 |
| | Mössbauer spectroscopy | | | | S30 |
| Applications | Typical devices based on HM DP oxides | Each device's performance | | | Ref. |
| | Magnetic tunnel junctions (MTJs) | A SFMO/STO/Co tunnel nanojunction measured at 4 K and applied bias voltage of 10 mV; TMR ~ 50%, negative spin polarization ($P$) of SFMO film, $P$ ~ - 85%, indicating the electron tunneling from SFMO through STO. | | | S31 |
| | Spin filtering devices (SFDs) based on tunnel jsctions | (a) Metallic/magnetic insulator/magnetic insulator/metallic (M-MI-MI-M) junctions or (b) ferromagnetic metal/nonmagnetic metal/magnetic insulator/ferromagnetic metal (FM-NM-MIFM) junctions; SFDs can operate at room temperature and exhibit magnetic field sensitivity much larger than conventional tunnel junctions conventional MTJs; TMR as high as $10^5$ predicted in a metal/spin filter 1/spin filter 2/metal structure ( double spin-filter junction) | | | S32 |

|  |  |  |  |
|---|---|---|---|
|  | Field effect transistors (FETs) | A spin MOSFET consisting of a MOS structure and half-metallic-ferromagnet (HMF) contacts for the source and drain; exhibiting high (low) current drive capability in the parallel (antiparallel) magnetization; extremely large magnetocurrent ratio $\gamma_{MC}$ (defined as $\frac{(I_D^P - I_D^{AP})}{I_D^{AP}}$) ($\gamma_{MC}$ > 1000% @$V_{DS}$ < 1.0 V) | S33 |
|  | Josephson junctions | HM ferromagnet-superconductor bilayers of $La_{0.7}Ca_{0.3}MnO_3$/ $Pr_{1.85}Ce_{0.15}CuO_4$ (LCMO/PCCO) grown by PLD on $NdGaO_3$ (001) substrates; long-ranged S-F proximity effects observed in the LCMO film (up to a distance much larger than for Cooper pairs in a singlet spin state to exist), which can be attributed to induced triplet-pairing correlations mediated by spin-active interfacial regions. | S34 |
|  | Applications in the field of electrocatalysts | Ir-based $Ba_2MIrO_6$ (e.g., M = Y, La, Ce, Pr, Nd and Tb) DP oxides synthesized by standard solid-state reactions, exhibiting tunable performance towards acidic OER. $Ba_2PrIrO_6$ is the best acidic OER electrocatalyst, surpassing the benchmark $IrO_2$. | S35 |
|  | Solid oxide fuel cells (SOFC) | $La^{3+}$-doped $Sr_2FeMoO_{6-\delta}$ (SLFM with 0≤x≤1) double perovskites used as anode materials for solid oxide fuel cells; SOFCs with SLFM(x=0.2) as anode have demonstrated excellent and stable performance under direct $CH_4$; the high catalytic activity for methane conversion of >99% at 800 °C. | S36 |

**Table S2**. The calculated methods used and the possible HM DP oxide systems as well as the experimentally verified examples.

| Calculation methods | Material systems | Calculation results | Experimentally verified | Ref. |
|---|---|---|---|---|
| Full-potential linearized augmented Plane wave (FPLAPW) | $Sr_2CrReO_6$ | Semiconductor to half-metal transition observed through 5% volume compression | Yes | S37 |
|  | $Sr_{2-x}La_xFe_{1+y/2}Mo_{1-y/2}O_6$ | Half-metal feature preserved in SLFMO for x = 1/2 and 1 contrary to the case for SFMO | Yes | S38, S39 |
|  | $Sr_2MoBO_6$ (B=W, Re, Os) | $Sr_2MoOsO_6$ is a compensated half metal | Yes | S40 |
|  | $La_2NbMnO_6$ | HM DP oxide | No | S41 |
|  | $Bi_2CuCrO_6$ | Doping with Pb, the system experiences a transition from A-type AFM phase to FiM phase | No | S42 |
| Full-potential linear muffin-tin orbital method (FPLMTO) | $Sr_2FeMoO_6$, $Sr_2FeReO_6$, $Sr_2CrWO_6$ | FiM HM DP oxides | Yes | S43 |
| Linearized Augmented Plane Waves method (LAPW) | $A_2FeMoO_6$ (A = Ca, Sr, and Ba) | Ferromagnetic oxides | Yes | S44, S45 |
|  | LaMM’$O_3$, MM’= MnCo, CrFe, CrRu, CrNi, MnV, and VCu | $La_2VMnO_6$, $La_2VCuO_6$ HM DP oxides | Yes, $La_2VMnO_6$,<br>Yes, $La_2VCuO_6$, | S46 |
|  | $(Ba_xSr_{1x})_2CoWO_6$ (x=0.1, 0.2, 0.3, 0.5, 0.7, and 0.9) | $Ba_2CoWO_6$ and $SrBaCoWO_6$ are half-metals | Yes | S47 |
| GGA+ U+SOC | $Pb_2FeOsO_6$ | Tetragonal *I*4/*m* structure and a C-type antiferromagnet | Yes | S48, S49 |
|  | $Sr_2BB'O_6$ (B= Cr, Mo, and B’ = W, Re, Os) | HM DP oxide | Yes | S50 |
|  | $Pr_{2-x}Sr_xMgIrO_6$ | x = 0.5 and 1.5 HM FiM DP oxide | No | S51 |
|  | $Ca_2AOsO_6$ (A = Cr, Mo) | when the volume is compressed to smaller than $0.9V_0$, $Ca_2MoOsO_6$ turns out to be a half metal | No | S52 |
|  | $La_2NiCrO_6$ | FM HM DP oxide | No | S53 |

| | | | | |
|---|---|---|---|---|
| GGA + U | $(Sr,Ca)_2BRhO_6$ (B = Cr, Mn, Fe) | Cr–Rh and Mn–Rh compounds predicted to be FM half-metals | No | S54 |
| | $Sr_{2-y}La_yFeMoO_6$ | FM HM DP oxides | Yes | S55 |
| | $Sr_2FeCoO_6$ | FM HM DP oxide | Yes | S56 |
| | $A_2CrRu(Os)O_6$ (A = Si, Ge, Sn, and Pb) | All its electronic structures convert HM-AF into unconventional AF-Is | No | S57 |
| | $Sr_2CoWO_6$ | FM and AFM phases calculated by GGA and GGA+U methods | Yes | S58 |
| | $La_2VCuO_6$, $La_2VTcO_6$ | HM AFM DP oxide | No | S59 |
| | $BaSrNiWO_6$ | FM or AFM states | Yes | S60 |
| | $Bi_2BB'O_6$ (B, B'= 3d transitional metals) | $Bi_2CrNiO_6$ and $Bi_2CrZnO_6$, HM DP oxides | No | S61 |
| | $Lu_2NiIrO_6$ | FiM HM DP oxides | Yes | S62 |
| | $Pb_2XX'O_6$ (X = Ti, Zr, Hf, V, Nb and Ta, X'= Tc, Ru, Os and Rh | $Pb_2NbTcO_6$, $Pb_2TaTcO_6$, $Pb_2TiRuO_6$, $Pb_2ZrRuO_6$, $Pb_2HfRuO_6$, $Pb_2VRuO_6$, $Pb_2NbRuO_6$, $Pb_2TadRuO_6$, $Pb_2ZrOsO_6$, $Pb_2HfOsO_6$, $Pb_2VOsO_6$, $Pb_2ZrRhO_6$ and $Pb_2HfRhO_6$ FiM HM DP oxides | No | S63 |
| | $Y_2CrMnO_6$ | HM DP oxide | Yes | S64 |
| | $La_2CrFeO_6$ | $La_{1.5}CrFeO_6$ behaves as half-metal with the half-metallic gap of 0.42 eV | Yes | S65 |
| Generalized gradient approximation (GGA) | $BiPbVRuO_6$ and $BiPbVOsO_6$ | HM-AFM DP oxides | No | S66 |
| GGA and GGA+U | $Ba_2DySbO_6$ | HM DP oxide | Yes | S67, S68 |
| GGA and GGA+U | $Sr_2BB'O_6$ (B, B' = 3*d* transition metal) | $Sr_2ScCrO_6$, $Sr_2TiCrO_6$, $Sr_2MnCrO_6$, $Sr_2ZnMnO_6$, and $Sr_2ZnFeO_6$ | $Sr_2ScCrO_6$, No<br>$Sr_2TiCrO_6$, Yes<br>$Sr_2MnCrO_6$, No<br>$Sr_2ZnMnO_6$, No<br>$Sr_2ZnFeO_6$, No | S69 |
| GGA and GGA+U | $Ba_2CdReO_6$ | FM HM DP oxide | Yes | S70 |
| GGA, GGA+U, GGA+SOC, and GGA+SOC+U | $Sr_2NiOsO_6$ | FM or AFM HM DP oxide | Yes | S71 |
| GGA, GGA-SOC | $Ba_2MnTeO_6$ | FM HM DP oxide | Yes | S72 |
| GGA + mBJ | $Ba_2FeNiO_6$ | 100% spin polarization | No | S73 |
| GGA-PBE | $Ba_2MMoO_6$ (M=Cr, Mn, Fe) | FM HM DP oxide | Yes | S74 |
| LSDA+U | $Ba_2CeCoO_6$ | FM HM DP oxide with space group of Fm3m | No | S75 |
| | $Sr_2CoMoO_6$ | From an AFM semiconductor to a half-metal | Yes | S76 |
| | $Ba_2FeMoO_6$ | HM DP oxide | Yes | S77 |
| LSDA+U | $K_2MnRhO_6$ and $La_2CrWO_6$ | Compensated half metals | No | S78 |
| LSDA and LSDA+U | $Sr_2Fe_{1-x}Cr_xReO_6$ (x = 0.0, 0.25, 0.5, 0.75, 1.0) | Cr doping from 3 $\mu_B$ for x = 0.0 down to 1.0 $\mu_B$ for x = 1.0 per formula unit | Yes | S79 |
| LDA | $Ba_2MMoO_6$ (M = Mn, Fe) | HM DP oxide | Yes | S80 |
| DFT +U | $Bi_2FeCrO_6$ | Doping to induce half-metal to insulator | Yes | S81 |
| | $Sr_2FeMoO_6$ | Antiferromagnets | Yes | S82 |
| | $La_2TiFeO_6$ | HM | Yes | S83 |
| DFT | $Ca_2Fe_{1-x}Ni_xOsO_6$ | x = 0.5, ferrimagnetism with $\mu_{tot} = 2\ \mu_B$/f.u. | Yes | S84, S85 |
| | $La_2FeMnO_6$ | FM HM DP oxide | Yes | S86, S87 |

## Reference

S1. P. Ksoll, C. Meyer, L. Schüler, V. Roddatis, V. Moshnyaga, *Crystals,* 2021, **11**, 734–753.

S2. S. Vasala, M. Karppinen, *Prog. Solid State Chem*., 2015, **43**, 1–36.

S3. V.M. Goldschmidt, *Naturwissenschaften,* 1926, **14**, 477–485.

S4. A. Bhattacharya, S.J. May, *Annu. Rev. Mater. Res*., 2014, **44**, 65–90.

S5. H. Kato, T. Okuda, Y. Okimoto, Y. Tomioka, Y. Takenoya, A. Ohkubo, M. Kawasaki, Y. Tokura. *Appl. Phys. Lett.*, 2002, **81**, 328–330.

S6. H. van Leuken, R.A. de Groot. *Phys. Rev. Lett.*,1995, **74**, 1171–1173.

S7. S. Biswas, S. Ram, *Chem. Phys.,* 2004, **306**, 163–169.

S8. Q. Zhao, Y. Fan, G. Wen, Z. Liu, H. Ma, X. Jia, G. Zou, H.K. Mao, *Mater. Lett.,* 2010, **64**, 592–595.

S9. S. Middey, S. Jana, S. Ray, *J. Appl. Phys.,* 2010, **108**, 043918.

S10. L. Fuoco, D. Rodriguez, T. Peppel, P.A. Maggard, *Chem Mater*., 2011, **23**, 5409–5414.

S11. X.H. Li, Y.P. Sun, W.J. Lu, R. Ang, S.B. Zhang, X.B. Zhu, W.H. Song, J.M. Dai, *Solid State Commun.,* 2008, **145**, 98–102.

S12. A.K. Azad, S.-G. Eriksson, A. Khan, A. Eriksson, M. Tseggai, *J. Solid State Chem.,* 2006, **179**, 1303–1311.

S13. C.R. Lin, Y.M. Chu, S.C. Wang, *Mater. Lett*., 2006, **60**, 2270–2273.

S14. X.Y. Li, Z.F. Yao, L.Y. Zhang, G.H. Zheng, Z.X. Dai, K.Y. Chen, *Appl. Surf. Sci.,* 2019, **480**, 262–275.

S15. M. Alam, K. Karmakar, M. Pal, K. Mandal, *RSC Adv*., 2016, **6**, 114722-114726.

S16. N. Kumar, R. Gupta, R. Kaur, D. Oka, S. Kakkar, S. Kumar, S. Singh, T. Fukumura, C. Bera, S. Chakraverty, *ACS Appl. Electron. Mater*., 2021, **3**, 597–604.

S17. H. Asano, Y. Kohara, M. Matsui, *Jpn. J. Appl. Phys.,* 2002, **41**, L1081–L1083.

S18. J. Rager, A.V. Berenov, L.F. Cohen, W.R. Branford, Y.V. Bugoslavsky, Y. Miyoshi, M. Ardakani, J.L. MacManus-Driscoll, *Appl. Phys. Lett*., 2002, **81**, 5003–5005.

S19. H. Kato, T. Okuda, Y. Okimoto, Y. Tomioka, K. Oikawa, T. Kamiyama, Y. Tokura, *Phys. Rev. B,* 2004, **69**, 184412.

S20. T.W. Lim, S.D. Kim, K.D. Sung, Y.M. Rhyim, H. Jeen, J. Yun, K.H. Kim, K.M. Song, S. Lee, S.Y. Chung, M. Choi, S.Y. Choi, *Sci. Rep*., 2016, **6**, 19746.

S21. Y. Moritomo, S. Xu, T. Akimoto, A. Machida, N. Hamada, K. Ohoyama, E. Nishibori, M. Takata, M. Sakata, *Phys. Rev. B,* 2000, **62**, 14224–14228.

S22. Y. Tomioka, T. Okuda, Y. Okimoto, R. Kumai, K.-I. Kobayashi, Y. Tokura, *Phys. Rev. B,* 2000, **61**, 422–427.

S23. Y. Moritomo, S. Xu, A. Machida, T. Akimoto, E. Nishibori, M. Takata, M. Sakata, K. Ohoyama, *J. Phys. Soc. Jpn.,* 2000, **69**, 1723–1726.

S24. D. Sanchez, J.A. Alonso, M. Garcıa-Hernandez, M.J. Martinez-Lope, M.T. Casais, J.L. Martinez, *J. Mater. Chem.,* 2003, **13**, 1771–1777.

S25. P. Tieu, X.X. Yan, M.J. Xu, P. Christopher, X.Q. Pan, *Small,* 2021, **17**, 2006482.

S26. G. Gorokh, A. Zakhlebayeva, A. Lazavenka, N. Sobolev, V. Zhylinski, N. Bogomazova, M. Yarmolich, N. Kalanda, *Phys. Status Solidi B,* 2020, **257**, 1900283.

S27. J.L. Hart, A.C. Lang, A.C. Leff, P. Longo, C. Trevor, R.D. Twesten, M.L. Taheri, *Sci. Rep.,* 2017, **7**, 8243.

S28. L. Yang, S. Fu, K. Leng, Q.K. Tang, Z.W. Wu, K. Yi, X.H. Zhu, *Open Ceram*., 2022, **9**, 100238.

S29. O. Mathon, P. van der Linden, T. Neisius, M. Sikora, J.M. Michalik, C. Ponchut, J.M. De Teresa, S. Pascarelli, *J. Synchrotron Rad.,* 2007, **14**, 409–415.

S30. M. Yarmolich, N. Kalanda, S. Demyanov, J. Fedotova, V. Bayev, N.A. Sobolev, *Phys. Status Solidi B,* 2016, **253**, 2160–2166.

S31. M. Bibes, K. Bouzehouane, A. Barthelemy, M. Besse, S. Fusil, M. Bowen, P. Seneor, J. Carrey, V. Cros, A. Vaures, J.-P. Contour, A. Fert, *Appl. Phys. Lett*., 2003, **83**, 2629–2631.

S32. M.G. Chapline, S.X. Wang, J. Appl. Phys. 2006, **100**, 123909.

S33. S. Sugahara, M. Tanaka, *Appl. Phys. Lett.,* 2004, **84**, 2307–2309.

S34. Y. Kalcheim, O. Millo, M. Egilmez, J.W.A. Robinson, M.G. Blamire, *Phys. Rev. B*, 2012, **85**, 104504.

S35. O. Diaz-Morales, S. Raaijman, R. Kortlever, P.J. Kooyman, T. Wezendonk, J. Gascon, W.T. Fu, M.T.M. Koper, *Nat. Commun.* 2016, **7**, 12363.

S36. X. Yang, J. Chen, D. Panthi, B.B. Niu, L.B. Lei, Z.H. Yuan, Y.H. Du, Y.F. Li, F.L. Chen, T.M. He, *J. Mater. Chem. A,* 2019, **7**, 733–743.

S37. J. Wang, N. Zu, Y. Wang, Z. Wu. Phys. *Status Solidi RRL*, 2013, **7**, 583–586.

S38. D. Stoeffler, *J. Phys. Conden.s Matter*, 2012, **24**, 046004.

S39. D. Rubi, *J. Appl. Phys.*, 2004, **95**, 7082–7084.

S40. N. Zu, L. Rui, Q. Li, J. wang, *J. Magn. Magn. Mater.*, 2016, **399**, 72–76.

S41. K.A. Parrey, S.A. Khandy, I. Islam, A. Laref, D.C. Gupta, A. Niazi, A. Aziz, S.G. Ansari, R. Khenata, S. Rubab, *J. Electron. Mater.*, 2018, **47**, 3615–3621.

S42. N. Zu, Q. Zhang, M. Zhang, J. Hao, X. Liu, R. Li, *J. Solid State Chem.*, 2021, **303**, 122521.

S43. H.T. Jeng, G.Y. Guo, *Phy. Rev. B*, 2003, **67**, 094438.

S44. C.M. Bonilla, D.A. Tellez, J.A.R. Martinez, J. Roa-Rojas, *Braz. J. Phys.*, 2006, 2006, **36**, 1101–1104.

S45. A. Isayama, S. Kadota, H. Yui, T. Sasagawa, *Mater. Sci. Eng. B*, 2010, **173**, 44–46.

S46. W.E. Pickett, *Phys. Rev. B*, 1998, **57**, 10613–10619.

S47. W. Wong-Ng, G.Y. Liu, D.D. Shi, Y.Q. Yang, R. Derbeshi, D. Windover, J.A. Kaduk, *Powder Diffr.*, 2020, **35**, 1–9.

S48. Ni. Zu, R. Li, W. Luo, D. Liu, X. Liu, Y. Liu, *J. Magn. Magn. Mater.*, 2019, **491**, 165553.

S49. Q. Zhao, M. Liu, J. Dai, H. Deng, Y. Yin, L. Zhou, J. Yang, Z. Hu, S. Agrestini, K. Chen, E. Pellegrin, M. Valvidares, L. Nataf, F. Baudelet, L.H. Teng, Y. Yang, C. Jin, Y. Long, *Inorg. Chem.*, 2016, **55**, 9816–9821.

S50. N. Zu, Q. Zhang, J. Hao, M. Zhang, J. Li, X. Liu, R. Li. *J. Solid State Chem.*, 2022, **312**, 123274.

S51. M.P. Ghimire, L.H. Wu, X. Hu, *J. Supercond. Nov. Mag.*, 2015, **28**, 917–919.

S52. N. Zu, R. Li, R. Ai, *J Magn. Magn. Mater.*, 2018, **467**, 145–149.

S53. J. Wang, X. Hao, Y. Xu, Z. Li, N. Zu, Z. Wu, F. Gao. *RSC Adv.*, 2015, **5**, 50913–50918.

S54. A. Halder, D. Nafday, P. Sanyal, T. Saha-Dasgupta, *npj Quantum Mater*., 2018, **17**, 1-8.

S55. A.M. Reyes, J.A. Montoy, O. Navarroa, *J. Magn. Magn. Mater.*, 2020, **495**, 165877.

S56. H.P. Wu, L.L. Wang, Y. Qian, W.S. Tan, C.Y. Xiao, K.M. Deng, *J. Appl. Phys.*, 2011, **110**, 083701.

S57. H. Fuh, Y.P. Liu, S.H. Chen, Y.K. Wang, *J. Alloy. Compd.*, 2013, **547**, 126–131.

S58. T. Hashemifar, A. Mokhtari, V. Soleimanian, *J Supercond. Nov. Magn*., 2017, **30**,497–503.

S59. Y.K. Wang, P.H. Lee, G.Y. Guo, *Phys. Rev. B*, 2009, **80**, 224418.

S60. Y. Aharbil, H. Labrim, S. Benmokhtar, M. A. Haddouch, L. Bahmad, A. Belhaj, H. Ez-Zahraouy, A. Benyoussef, *Mater. Chem. Phys.*, 2016, **183**, 588–594.

S61. H.Z. Lin, C.Y. Hu, P.H. Lee, A.Z. Yan, W.F. Wu, Y.F. Chen, Y.K. Wang, *Materials,* 2019, **12**, 1844.

S62. S. Nazir, *Sci. Rep.,* 2021, **11**, 1240.

S63. B.Y. Chen, P.H. Lee, Y.K. Wang, *Materials*, 2022, **15**, 3311.

S64. W. Wang, F. Liu, X. Zhang, X. Shen, Y. Yao, Y. Wang, B. Liu, X. Liu, R. Yu, *Inorg. Chem. Front*., 2018, **5**, 217–224.

S65. H. Wu, Y. Qian, W. Tan, E. Kan, R. Lu, K. Deng, *Phys. Lett. A*, 2015, **379**, 2897–2901.

S66. K.C. Weng, Y.K. Wang, *J. Phys. Soc. Jpn.*, 2014, **83**, 054715.

S67. D. Jha, G. Mandal, C. Ray, A.K. Himanshu, B.K. Singh, U. Kumar, B.K. Choudhary, *AIP Conf. Proc.*, 2016, **1731**, 090036.

S68. C. Vijayakumar, H. Padma Kumar, V.T. Kavitha, S. Solomon, J.K. Thomas, P.R.S. Wariar, J. Koshy, *J. Alloy. Compd.*, 2009, **475**, 778–781.

S69. Y.P. Liu, S.H. Chen, J.C. Tung, Y.K. Wang, *Solid State Commun.*, 2012, **152**, 968–973.

S70. S.A. Khandy, S. Yousuf, T.M. Bhat, S. Singh, S.A. Sofi, S.A. Mir, A.Q. Seh, M. Nabi, N.A. Ganie, A. Rasool, R.A. Mir, P. Kumar, D.C. Gupta, *AIP Conf. Proc.*, 2020, **2265**, 030359.

S71. W. Song, E. Zhao, J. Meng, Z. Wu, *J. Chem. Phys.*, 2009, **130**, 114707.

S72. H.M. Huang, Q. Yu, R. Tong, C.R. Wu, Z.W. Zhu, Z.D. He, S.J. Luo, *Results Phys.*, 2021, **25**, 104315.

S73. S.A. Mir, D.C. Gupta, *Sci. Rep.*, 2021, **11**, 10506.

S74. N.A. Shahed, M. Nishat, S. Khanom, M.K. Hossain, M.A. Hossain, F. Ahmed, *Comput.Condens. Matter*, 2020, **23**, e00464.

S75. H.H. Xie, Q. Gao, L. Li, G. Lei, X.R. Hu, J.B. Deng, *Solid State Commun.*, 2016, **239**. 49–54.

S76. C. Liu, W. Wan, S. Gong, H. Zhang, W. Guo, *Sci. Rep.*, 2017, **7**, 3856.

S77. J.S. Kang, J.H. Park, B.W. Lee, B.I. Min, *J. Phys. Soc. Jpn.,* 2002, **71**, 157–159.

S78. V. Pardo, W.E. Pickett, *Phys. Rev. B*, 2009, **80**, 054415.

S79. Q.F. Li, X.F. Zhu, L.F. Chen, *Phys. Lett. A*, 2008, **372**, 2911–2916.

S80. N.A. Shahed. M.K. Hossain, S. Khanom, M. Nishat, M.J. Alam, M.A. Hossain, F. Ahmed, *SPIN*, 2020, **10**, 2050023.

S81. P.C. Rout, V. Srinivasan, *Phys. Rev. Lett*., 2019, **123**, 107201.

S82. N. Kumar, R. Gupta, R. Kaur, D. Oka, S. Kakkar, S. Kumar, S. Singh, T. Fukumura, C. Bera, S. Chakraverty, *ACS Appl. Electron. Mater*., 2021, **3**, 597–604.

S83. E. Fertitta, S. Das, D. Banerjee, F. Ebrahimi, C. Barraud, K. Du, H. Tian, C.J. Pickard, C. Weber, R. Ramesh, P. Littlewood, D. Dubbink, *npj Comput. Mater.,* 2021, **92**, 1-8.

S84. M.P. Ghimire, X. Hu, *Mater. Res. Express*, 2016, **3**, 106107.

S85. H.L. Feng, M. Arai, Y. Matsushita, Y. Tsujimoto, Y. Guo, C.I. Sathish, X. Wang, Y.H. Yuan, M. Tanaka, K. Yamaura, *J. Am. Chem. Soc*., 2014, **136**, 3326–3329.

S86. Y. Qian, H. Wu, E. Kan, J. Lu, R. Lu, Y. Liu, W. Tan, C. Xiao, K. Deng, *J. Appl. Phys.*, 2013, **114**, 063718.

S87. M. Nasir, M. Khan, S.A. Agbo, S. Bhatt, S. Kumar, S. Sen, *J. Phys. D: Appl. Phys.*, 2020, **53**, 375003.