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Defect formation, magnetic interaction and electron phonon coupling in iron selenides $\mathbf{M_{1-x}Fe_{2-y}Se_2}$ XUHUI LUO, University of Illinois at Chicago & National Institute of Standard and Technology, SERDAR OGUT, University of Illinois at Chicago, TANER YILDIRIM, National Institute of Standard and Technology & University of Pennsylvania — We perform a systematic study to explore the electronic and magnetic structures in iron selenide superconductors $M_{1-x}Fe_{2-y}Se_2$ using first principles calculations. We show that there is an intimate relationship between Se-height and the underneath Fe-spin square in $M_{1-x}Fe_{2-y}Se_2$. A displacement of the Se atom by as small as 0.2Å is enough to change the amount of charge in the Fe-plane as much as 0.7 e per Fe. The Se-height increases as the number of ferromagnetic Fe-Fe bonds increases, yielding an expansion of 2Å expansion in the c-axis for fully ferromagnetic spin configuration, which indicates a giant magneto-elastic coupling in these systems. Our calculations also explain why the formation of Fe vacancies is favorable in iron selenides, but not in iron pnictides. Finally, we calculate the spin-resolved electron-phonon coupling in MFe_2Se_2 and $M_{1-x}Fe_{2-y}Se_2$ to shed light on the mechanism of superconductivity in these materials.

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