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First-principles Study of Electronic Structures and Phonons in $\mathbf{FeSe_{1-x}}$ ANIL KUMAR, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, AJAY K. SOOD, Indian Institute of Science, Bangalore, India, UMESH V. WAGHMARE, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India — We present first-principles density functional theory based calculations to assess the effects of Se vacancies (which are essential for the material to be superconducting) and strength of on-site correlation on (a) phonon frequencies, and (b) electronic density of states of the non-magnetic and different magnetic phases of $FeSe_{1-x}$. Our calculations show that energetically anti-ferromagnetic stripe ordering is favorable compared to the non-magnetic and other magnetic phases. We also find that the phonon frequencies are quite sensitive to the vacancies, magnetic ordering and on-site correlation parameter U, and interpret these results in terms of spin-spin and spin-phonon couplings. Our estimate of the spin-phonon coupling is comparable to the superconducting transition temperature of FeSe. The presence of Se vacancies in the system results in a large peak in the density of states near the Fermi level, which possibly enhances the superconducting transition temperature.

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