Composition and temperature dependent electronic structures of $NiS_{2-x}Se_x$ alloys: First-principles dynamical mean field theory approach

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We investigate the evolution of the electronic structure of $NiS_{2-x}Se_x$ alloys with varying the temperature and composition x using the combined approach of density-functional theory and dynamical mean-field theory. Adopting realistic alloy structures containing S and Se dimers, we map their electronic correlation strength on the phase diagram and observe the metal-insulator transition (MIT) at the composition x = 0.5, which is consistent with the experimental measurements. The temperature dependence of the local magnetic susceptibility is found to show a typical Curie-Weiss-like behavior in insulating phase while a constant Pauli-like behavior in metallic phase. The comparison of the electronic structures for NiS_2 and $NiSe_2$ in different lattice structures suggests that the MIT in this alloy system can be classified as a bandwidth-control type, where the change of the hybridization strength between Ni d and chalcogen p orbitals is the most important parameter.