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The optical, electronic and magnetic properties of Fe based binaries and diluted alloys AHMAD ALSAAD, Department of Physics, Jordan University of Science & Technology, ISSAM ALQATTAN. DEPARTMENT OF APPLIED MATHEMATICS AND SCIENCES TEAM — The optical, electronic, and magnetic properties of binaries and alloys containing small amount of iron (Fe) have been presented. In particular, diluted Fe alloys have been examined by several experimental techniques such as magnetization measurements, nuclear magnetic resonance or neutron scattering. Theoretically, the understanding of diluted Fe alloys has not been yet satisfactorily studied. We present *ab initio* calculations based on Local Density Approximation of Density Functional Theory for Fe based binaries and Fe lightly doped alloys (not to exceed 10%) with *3d* and *4d* transition elements. Results on the densities of states, the local magnetic moments, and the electronic specific heat around the *3d* and *4d* impurities have been reported. Contrary to the case of Co, Mn, and Ni alloys. Our density of states results indicate that most of the optical, electronic and magnetic properties of Fe alloys is attributed to the majority-spin states rather than the minority-spin states. This arises from the fact that the Fermi energy falls into the minimum of the minority-spin density of states rather than the minimum of the majority-spin states. The mechanism behind this very complicated magnetic behavior of Fe based binaries and alloys have been addressed and explained. The comparison between our theoretical results and the available experimental results will be presented.

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