Abstract Submitted
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Magnetism of Mn doped in a-Si and a-Ge[1] JUEXIAN CAO — With experimental studies and density function theory calculations, we report on the properties of Mn-doped amorphous Si and Ge which are designed to understand the fundamentals of cooperative phenomena in highly correlated electronic and magnetic systems. We observed a striking difference in Mn local moment when doped in $a-$Si and $a-$Ge matrices, in great contrast to the previous speculation that these two should behave very similar as the semiconductor host for transition metals. While we observed a large local moment of Mn in $a-$Ge, Mn moment is quenched in $a-$Si. The large difference of local magnetic moment of Mn in $a-$Si and $a-$Ge can be understood by the local atomic environment at the magnetic dopant sites, that is, the bond length and the coordination. Statistical DFT calculations shows that the magnetic dopant Mn with less coordination and large bond length hold large magnetic moment. Otherwise, the magnetic moment would be killed. In $a-$Ge, dopant Mn favours less coordination and large bond while more coordination and small bond length in $a-$Si, which result in the enhancement/quenchement of local magnetic moment Mn in $a-$Si/$a-$Ge.

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