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**Magnetic Main Group Impurities in CdS** PEDRO BEDOLLA-VELAZQUEZ, CHRISTOPH GRUBER, PETER MOHN, Vienna University of Technology — With the development of magnetic semiconductors, the role of the magnetism of impurities came again into the focus of research. For *d*- and *f*-electron impurities, the situation seems to be rather clear. A new field appears when one starts to study magnetism produced by vacancies or by atoms, which usually do not carry any magnetic moments in a bulk solid. Starting from the magnetism of carbon vacancies in graphene we will present a study of CdS where S is replaced by main group elements. On the basis of abinitio supercell calculations employing density functional theory (DFT) we investigate the behaviour of impurities (B, N, C, O, F, Al, Si, P, Ga, Ge) in wurtzite (w) and zinblende (zb) CdS lattices. It is found that the impurities prefer the sulfur position and most of them, depending on the concentration exhibit magnetic order. We find that for small concentrations (64zb/72w and 32zb atom supercells) a half metallic ferromagnetic behaviour is found. For a 16 atom supercell for both zb and wstructure partly also unsaturated magnetic moments occur. A field dependence of the magnetic moments in these materials may lead to new technological applications in these magnetic semiconductors as tunable spin injection materials.

Prefer Oral Session  
 Prefer Poster Session

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