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Rocksalt MnN: A Vacancy Stabilized Structure MAOSHENG MIAO, WALTER LAMBRECHT, Department of Physics, Case Western Reserve University — Recent density functional computations showed that the zinc blende is the most stable structure for MnN. However, so far MnN has only been found in a tetragonally distorted rocksalt (RS) structure. This conflict is resolved by our full potential linearized muffin-tin orbital calculations that showed the RS structure is stabilized by a few percent of nitrogen vacancies in MnN. Our calculations show that that the Gibbs energy of formation of the vacancy is low even under quite N-rich conditions and can even be negative under N-poor conditions. On the other hand, vacancies are hard to form in the ZB structure. The vacancies also affect the magnetic moments of their surrounding Mn atoms. When several vacancies are introduced per supercell we find that in the RS structure the vacancies prefer to stay in next nearest neighbor positions from each other at low concentration while they form ordered structure at high concentration. For the ZB structure, the vacancies tend to stay close even at high concentration. Supported by ONR and NSF.

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