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**Rocksalt MnN: A Vacancy Stabilized Structure**

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tions 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 calcu-  
lations 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.  
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