

Abstract Submitted  
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**A New Boundary Condition for Embedding Atoms in Solids**

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97403-1274 — Previously, Haydock and Nex [Phys. Rev. B 82, 205114 (2010)] for-  
mulated an approximation for embedding a finite discrete system into an infinite  
substrate by means of a new boundary condition. This boundary condition requires  
a maximum breaking of time-reversal symmetry (MBTS) in the sense that proba-  
bility is carried away from the embedding surface at a maximal rate. The MBTS  
boundary condition has been useful in discrete systems for constructing accurate  
densities of states and other distributions from moments or continued fractions. In  
this work, we generalize the approach to the problem of embedding an atom or a  
cluster of atoms into an infinite solid. The new, continuous MBTS boundary condi-  
tion has been applied to model systems and to the embedding of a hydrogen atom.  
Results are presented and compared with other methods.

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