

Abstract Submitted  
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**Understanding cation ordering and oxygen vacancy site preference in  $\text{Ba}_3\text{CaNb}_2\text{O}_9$  from first-principles**<sup>1</sup> HEPENG DING, ANIL VIRKAR, FENG LIU, University of Utah — We investigate the physical mechanism underlying the formation of the B-site cation ordering and the oxygen vacancy site selection in  $\text{Ba}_3\text{CaNb}_2\text{O}_9$  using density functional theory calculations. We found that either cation site exchange or oxygen vacancy formation induces negligible lattice strain. This implies that the ionic radius plays an insignificant role in governing these two processes. Furthermore, the electrostatic interactions are found dominant in the ordering of mixed valence species on one or more sites, the ionic bond strength is identified as the dominant force in governing both the 1:2 B-site cation ordering along the  $\langle 111 \rangle$  direction and the oxygen vacancy site preference in  $\text{Ba}_3\text{CaNb}_2\text{O}_9$ . Specifically, the cation ordering can be rationalized by the increased mixing bonding energy of the Ca-O-Nb bonds over the Ca-O-Ca and Nb-O-Nb bonds, i.e.,  $1/2(\text{Ca-O-Ca} + \text{Nb-O-Nb}) < \text{Ca-O-Nb}$ ; while oxygen vacancy prefers a site to minimize the electrostatic energy and to break the weaker B-O-B bond.

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Hepeng Ding  
University of Utah

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