

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Effect of band filling and symmetry breaking on the electronic ground state in  $(\text{LaXO}_3)_2/(\text{LaAlO}_3)_4(111)$  ( $X = 3d$ ) superlattices<sup>1</sup>** DAVID DOENNIG, FRM II, TU Munich, WARREN E. PICKETT, University of California at Davis, ROSSITZA PENTCHEVA, University of Duisburg-Essen — Structural patterns, e.g. a buckled honeycomb lattice, realized in (111)-oriented perovskite bilayers may lead to exotic electronic ground states such as a Dirac-point Fermi surface [1-3]. Based on density functional theory calculations including a Hubbard  $U$  term, we explore systematically the effect of band filling in [111]-oriented  $(\text{LaXO}_3)_2/(\text{LaAlO}_3)_4$  superlattices with  $X$  spanning the series of open shell  $3d$  ions. The interplay of charge, spin, orbital, and lattice degrees of freedom reveals some regularities over the series, but also several unexpected symmetry lowering reconstructions that can guide the design of artificial materials of desired spin-charge-orbital order in conjunction with size of the energy gap and the possibility for emergent topological character.

[1] D. Xiao, et al., Nat. Commun. **2**, 596 (2011).

[2] D. Doennig, W. E. Pickett, and R. Pentcheva, Phys. Rev. Lett. **111**, 126804 (2013).

[3] D. Doennig, W. E. Pickett, and R. Pentcheva, Phys. Rev. B **89**, 121110(R) (2014).

<sup>1</sup>Financial support by DFG SFB/TR80, project G3.

Rossitza Pentcheva  
University of Duisburg-Essen

Date submitted: 14 Nov 2014

Electronic form version 1.4