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Shell model for $BaTiO_3$-$Bi(Zn_{1/2}Ti_{1/2})O_3$ perovskite solid solutions J. VIELMA, D. JACKSON, D. ROUNDY, G. SCHNEIDER, Oregon State University — Even though the composition of $BaTiO_3$-$Bi(Zn_{1/2}Ti_{1/2})O_3$ perovskite solid solutions is similar to other ferroelectric compounds, the dielectric response is unusual. Results of permittivity measurements as a function of temperature show a diffuse phase transition indicative of a weakly coupled relaxor behavior.[1] To investigate the weakly coupled relaxor behavior in these materials at intermediate length scales we are developing a newly calibrated shell model based on first-principles supercell calculations of both the solid solution and its compositional endpoints. Initial results for its phase diagram will presented.

[1]C. C. Huang and D. P. Cann, J. Appl. Phys. **104**, 024117 (2008)

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