correspond to configurations with the same λ value (e.g., $\lambda = 1$) their E_1 and E_2 terms have exactly the same value and the relative electrostatic energy equals the difference only between the E_3 terms, that is, $E_{PIE}(\blacktriangleleft_1) - E_{PIE}(\blacktriangleleft_2) = E_3(\blacktriangleleft_1) - E_3(\blacktriangleleft_2)$. Since the sum in E_3 runs only over cations, $E_3(\blacktriangleleft_1, \blacktriangleleft_2)$ does not depend at all on the oxygen displacement parameter u. In that case,

$$E_{PIE}(\blacktriangleleft_1, \blacktriangleleft_2$$

on 50 randomly chosen inverse configurations out of 2987 with up to 56 atoms. All DFT calculations are performed with the PBE exchange−correlation functional,[22] within the projected augmented wave method[23] as implemented in VASP.[24] The density of the Monkhorst−Pack k-point mesh[25] is kept constant to the value corresponding to the $6 \times 6 \times 6$ mesh for the 14-atom primitive cell of the normal spinel structure. The plane wave cutoff of 400 eV is used.

The results shown in Figure 3b demonstrate the regression $E_{DFT}(\blacktriangle) = 1/ E_{PIE}(\blacktriangle, = 1) + $ between PIE and DFT energies computed by taking the $P4_1 22$ structure as a reference. The value of the lattice constant a, the input parameter to the PIE model, is taken from experiments,[26−28] whereas in the DFT calculations all lattice vectors and the atomic positions have been relaxed to equilibrium. The fitted value of is equal to zero in all

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dx.doi.org/10.1021/ja2034602 |*J. Am. Chem. Soc.* 2011, 133, 11649–11654

There are two important implications of the regression of E_{PIE} and E_{DFT}: (i) to a good approximation, there is a universal scalability between E_{DFT} for different compounds, and (ii) Since 2-4 spinels have approximately up to 2 times bigger values than 3-2 spinels [= 13.6 (Zn_2SnO_4) and = 18.5 (Zn_2VO_4) for the 2-4 cases, while = 9.8 (Al_2NiO_4) and = 11.1 (Ga_2MgO_4) for the 3-2 spinel oxides], the scaling factor Z_r^2/a is 2−