

Abstract Submitted  
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**New metastable (Hf,Zr)O<sub>2</sub> phases: are the traditional structure prediction methods good enough?** SERGEY BARABASH, Intermolecular Inc. — The recent discovery of ferroelectric and antiferroelectric behavior in (Hf,Zr)O<sub>2</sub>-based films[1] has further highlighted the paramount industrial importance of stabilizing metastable phases in (Hf,Zr)O<sub>2</sub>, already sought for the outstanding dielectric properties. Potentially, together with the phases that are also observed at high temperatures or in strongly doped” materials, yet-unknown phases may also be stabilized. In fact, prior theoretical studies[2,3] have predicted several such possible new phases. Here we demonstrate that there is, in fact, a much larger number of potential metastable (Hf,Zr)O<sub>2</sub> phases, including several yet-unknown phases exhibiting ferroelectric properties. Many of the phases predicted here have quite low formation energies, yet were missed in previous studies. We discuss the challenges encountered by the earlier structure searches in (Hf,Zr)O<sub>2</sub>, and offer an alternative methodology more appropriate to predict possible metastable structures in such systems. [1] M.H. Park et al., *Adv.Mater.* **27**, 1811 (2015), and references therein. [2] T.D. Huan et al., *Phys. Rev.B* **90**, 064111 (2014). [3] Q.Zeng et al., *Acta Cryst. C* **70**, 76 (2014).

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