

Abstract Submitted  
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**Microscopic origin of pressure-induced phase transitions in iron pnictides**<sup>1</sup> INGO OPAHLE, YU-ZHONG ZHANG, Institut fuer Theoretische Physik, Unversitaet Frankfurt, HEM C. KANDPAL, Leibniz Institute for Solid State and Materials Research Dresden, HARALD O. JESCHKE, ROSER VALENTI, Institut fuer Theoretische Physik, Unversitaet Frankfurt — We have performed ab initio molecular dynamics calculations on the three materials (Ca, Sr, Ba)Fe<sub>2</sub>As<sub>2</sub> under pressure. We find that the structural phase transition (orthorhombic to tetragonal symmetry) is always accompanied by a magnetic phase transition in all the compounds, while the nature of the transitions is different for the three systems. Our calculations explain the origin of the existence of a collapsed tetragonal phase in CaFe<sub>2</sub>As<sub>2</sub> and its absence in BaFe<sub>2</sub>As<sub>2</sub>. We will also present a detailed analysis of pressure-induced superconductivity in BaFe<sub>2</sub>As<sub>2</sub> based on neutron diffraction experiments, ARPES and bandstructure calculations and we will show the importance of structural distortions for the onset of superconductivity.

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Harald O. Jeschke  
Institut fuer Theoretische Physik, Unversitaet Frankfurt

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