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# Pretransitional dynamics in prototype antiferroelectric material PbZrO3

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Lead zirconate (PZO) has been recently a subject of intensive studies with its antiferroelectric (AFE) phase transition (PT) being in a spotlight. Since there is no direct link between the paraelectric cubic phase and the low temperature orthorhombic one, the process leading to the emergence of AFE order is not obvious. Results of X-ray inelastic as well as Brillouin scattering experiments has directed Tagantsev et al. to propose a flexoelectric coupling to be the main physical mechanism behind the AFE PT [1]. On the other hand, Hlinka et al. on the basis of infra-red, Raman and THz spectroscopy as well as group theory considerations proposed an alternative picture of the PT mechanism where soft ferroelectric branch is coupled by a trilinear term to two oxygen octahedra tilt modes [2].
We present a shell model molecular dynamics study of PZO. This recently developed model has already been used for explanation of X-ray [3] as well as neutron diffuse scattering data [4]. Very good agreement between modeled and experimental intensities (coming mostly from phonons) assures that the model correctly describes dynamics of the system. The atomistic simulation allows us to study theoretically phonons at finite temperatures (for the first time for PZO). To shed the light on the emergence of the AFE order, we concentrate on the cubic phase and show how the lattice dynamics changes towards the phase transition.

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