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Atomic dynamics in PrBaCo2O6 ELVIS SHOKO, UDO SCHWINGENSCHLOGL, King Abdullah University of Science and Technology,Thuwal, 23955-6900 — We have used a combination of lattice dynamics and *ab initio* molecular dynamics (MD) to study atomic dynamics in $PrBaCo_2O_6$, a prototype material for a large class of layered compounds of both fundamental and technological interest. With the layered structure as the framework for understanding the dynamics, our analysis reveals clear signatures of this structural motif in the overall atomic dynamics, especially for O atoms. In particular, we find that O atom dynamics in the PrO layer is predominantly in-plane (*ab*-plane) in contrast to the predominantly out-of-plane dynamics in the CoO_2 layer. This finding suggests that the oxide ionic conductivity is dominated by the O atoms in the PrO layer. Additionally, we find sharp low-energy modes below 20 meV for both Ba and Pr atoms, reminiscent of rattler modes known for reducing thermal conductivity in cage compounds.

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