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Microscopic Picture of Atomic Dynamics in the Double Perovskite, $PrBaCo_2O_6$ ELVIS SHOKO, UDO SCHWINGENSCHLOGL, PSE Division, KAUST, Saudi Arabia — We have used a combination of lattice dynamics and *ab initio* molecular dynamics to study atomic dynamics in $PrBaCo_2O_6$, a prototype material for a large class of layered compounds of both fundamental and technological interest. We find clear signatures of the layered structure of this compound on the overall atomic dynamics. 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 suggests that the oxide ionic conductivity is dominated by the O atoms in the PrO layer, a finding of interest in solid-oxide fuel cells. Additionally, our results reveal sharp low-energy vibrational modes below 20 meV for both Ba and Pr atoms leading to the intriguing possibility that this material may be engineered for thermoelectric applications.

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