## ab initio calculations reveal why thermal and compositional variations are required to explain observed mantle shear and compressional velocity anomalies

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The sensitivity of seismic velocity and density to composition and temperature determines the ability to detect changes in these properties in the lower mantle. We use recent ab initio calculations to predict the sensitivity of shear, bulk, and compressional velocity and density to changes in composition and temperature under lower mantle conditions. We calculate the predicted seismic signals for a suite of compositions and temperatures. These predictions are then compared to seismic tomography observations. If only shear velocities are used, the magnitude of observed seismic anomalies can be matched by varying temperature alone for any single composition. However, the compressional velocity sensitivity to temperature and composition is complex, in part due to the effects of the iron high spin to low spin transition in ferropericlase. We find it is essentially impossible to account for the observed magnitude of both shear and compressional velocities in a homogeneous mantle. Lateral and/or vertical gradients in composition are required to explain the fundamental properties of almost all joint tomography models.

Keywords: seismic tomography, mantle state and composition