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High Temperature Thermal Conductivity from First Principles CHRISTIAN CARBOGNO, Materials Department, University of California Santa Barbara / Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, RAMAMURTHY RAMPRASAD, University of Connecticut, Storrs / Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — In spite of significant research efforts, little is yet known about the atomistic details and mechanisms that underlie peculiarly low (or high) thermal conductivities, especially at elevated pressures and temperatures. Under such extreme conditions, systematic experimental measurements are hard to perform; conventional theoretical approaches typically fail to capture significant physical aspects of the problem, since these methods are either inherently limited to (a) low temperatures and/or (b) to perfect crystals. A recently developed *ab initio* simulation strategy [1] allows to overcome the latter limitation, but the assessment of the high temperature regime remains an unsolved challenge. Within this work, we present efficient strategies to overcome this serious restriction and show their applicability for zirconia based ceramics - a material typically used in high temperature applications, for instance in thermal barrier coatings [2].
[1] T. M. Gibbons, and S. K. Estreicher, *Phys. Rev. Lett.* **102**, 255502 (2009).
[2] D. R. Clarke, and C. G. Levi, *Annu. Rev. Mat. Res.* **33**, 383 (2003).

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