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Thermomechanical properties in the AFLOW distributed database CORMAC TOHER, COREY OSES, JOSE J. PLATA, DAVID HICKS, FRISCO ROSE, OHAD LEVY, Dept. of Mechanical Engineering and Materials Science, Duke University, Durham, NC, MAARTEN DE JONG, MARK ASTA, Dept. of Materials Science, UC Berkeley, CA, OLEXANDR ISAYEV, ALEXANDER TROPSHA, School of Pharmacy, UNC, Chapel Hill, NC, MARCO FORNARI, Dept. of Physics, Central Michigan University, Mount Pleasant, MI, MARCO BUONGIORNO NARDELLI, Dept. of Physics, Univ. of North Texas, Denton, TX, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, Durham, NC — The integrated AEL-AGL workflow [1] has been used to automatically calculate the thermal and elastic properties for over 3000 materials in the AFLOW computational materials data repository [2, 3, 4]. This data set can be used in combination with the AFLOW Search API to screen for candidate materials for applications such as thermoelectrics, heat sinks and thermal barrier coatings. The data set has also been used to train machine learning models for thermomechanical properties, which has been successfully used to predict properties including the bulk modulus and the Debye temperature for tens of thousands of materials. [1] C. Toher et al., Phys. Rev. B 90, 174107 (2014). [2] S. Curtarolo et al., Comp. Mat. Sci. 58, 218 (2012). [3] S. Curtarolo et al., Comp. Mat. Sci, 58, 227 (2012). [4] http://aflow.org/

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