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Effects of disorder on the T-dependent bandstructure of purple bronze $Li_2Mo_{12}O_{34}$ THOMAS JARLBORG, PIOTR CHUDZINSKI, THIERRY GIAMARCHI, DPMC, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland — The band structures of ordered and disordered $Li_2Mo_{12}O_{34}$ are calculated by use of ab-initio DFT-LMTO method. The unusual band dispersion in the z-direction obtained in previous band calculations is confirmed for the ordered structure, and the overall band structure agree reasonably with existing photoemission data. The T-dependent band broadening is calculated from configurations with thermal disorder of the atomic positions within the unit cell. The band structure shows important band broadening of the two bands at the Fermi energy. The bands are particularly sensitive to in-plane movements of Mo sites. Already disorder due to zero-point motion makes a band broadening of the order of 20 meV and creates a sizable band overlap. The effect of Li vacancies on the two bands is relatively small.

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