Metallic nitrogen at high pressure and temperature\textsuperscript{1} BRIAN BOATES, Dalhousie University, STANIMIR BONEV, Dalhousie University, Lawrence Livermore National Laboratory — A polymeric, metallic phase of solid nitrogen is predicted at high pressure and temperature from first principles. The structure is found using a novel approach that makes use of structural information from simulations of liquid nitrogen in an effort to incorporate already known finite-temperature behavior. We have determined the finite-temperature phase boundaries of several competitive phases and report results for the conductivity of both solid and liquid nitrogen. Routes for experimental detection of the new structures are proposed.

\textsuperscript{1}Work supported by NSERC, the Killam Trusts, ACEnet, and LLNL. Prepared by LLNL under Contract DE-AC52-07NA27344.