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Mechanical, optoelectronic and transport properties of single-layer Ca_2N and Sr_2N electrides

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Abstract

Electride materials offer attractive physical properties due to their loosely bound electrons. Ca_2N , an electride in the two-dimensional (2D) form was successfully recently synthesized. We conducted extensive first-principles calculations to explore the mechanical, electronic, optical and transport response of single-layer and free-standing Ca_2N and Sr_2N electrides to external strain. We show that Ca_2N and Sr_2N sheets present isotropic elastic properties with positive Poisson's ratios, however, they yield around 50% higher tensile strength along the zigzag direction as compared with armchair. We also showed that the strain has negligible effect on the conductivity of the materials; the current in the system reduces by less than 32% for the structure under ultimate uniaxial strain along the armchair direction. Compressive strain always increases the electronic transport in the systems due to stronger overlap of the atomic orbitals. Our results show that the optical spectra are anisotropic for light polarization parallel and perpendicular to the plane. Interband transition contributions along in-plane polarization are not negligible, by considering this effect the optical properties of Ca_2N and Sr_2N sheets in the low frequency regime significantly changed. The insight provided by this study can be useful for the future application of Ca_2N and Sr_2N in nanodevices.

Keywords: Ca_2N and Sr_2N ; 2D electride; mechanical; electronic; optical

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