Spontaneous off-stoichiometry as the knob to control dielectric properties of La_3Te_4

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The properties of any given material are defined by atomic identities, composition, and structure (ACS). This implies that the design of a material with a target functionality requires identifying specific ACS accommodating specific material properties, and unless such materials are identified, the optimal device performance cannot be reached. For instance, for solar cell materials, a difference in band gap energy of 0.1 eV can be essential to change the theoretical limit (Shockley–Queisser limit) by a few percent. Such robust functionality depends on ACS leads to a situation when identifying a knob to tune given properties (e.g., dielectric properties) became the crucial task of material design. For instance, by adjusting the knob, the screened plasma frequency (frequency at which $\varepsilon_1(\omega)$ is equal to zero) can be tuned to optimize the material's performance for a particular application (e.g., metamaterials [1], epsilon-near zero materials [2]). Here, we demonstrate that La_3Te_4 (a representative example of a wide class of gapped metal compounds) can develop spontaneous off-stoichiometry due to the decay of conduction electrons to the acceptor level. Such behavior can form a range of non-stoichiometric compounds with the same parental crystal structure decorated by La vacancies, and tunning synthesis conditions can be used to stabilize target composition with desired electronic properties [3] and target dielectric properties.

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