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The Real Modulated NdTe₃ Structure Type and its Properties: A Combined Superspace Group / Pair Distribution Function Analysis Approach. Christos Malliakas,¹ HyunJeong Kim,² Daniel Bilc,² Simon Billinge,² Bhanu Mahanti,² Mercouri G. Kanatzidis,¹ ¹Dept. of Chemistry and Center for Fundamental Materials Research, ²Dept. of Physics and Astronomy, Michigan State Univ., East Lansing, MI 48824.

The structures of the rare earth trichalcogenides REQ₃ (Q=Se, Te) have been known since the 60s. These compounds crystallize in the so-called NdTe₃ structure type in space group Cmc. The structure consists of puckered [NdTe] double slabs, and layers of tellurium made of “perfect” square planar Te atoms stacked in the order –[NdTe]–[Te]–[Te]–. A closer look in these nets shows that there is a distortion and formation of a superstructure with respect to the ideal square net. Compounds with these features can give rise to interesting physical properties such as charge density waves.

Single crystal x-ray intensity data of RETe₃ compounds (RE=La, Ce, Pr, Nd, Sm, Gd) have been collected. We have solved the modulated structures using both 3D conventional crystallography and the 4D superspace approach (q-vector). We have confirmed the resulting crystal structures as being representative of the total bulk crystals using synchrotron radiation and pair distribution function (PDF) analysis. Details on the data collection and different techniques will be presented. Electronic and charge transport properties will be also presented.