## Abstract

This paper contains the comparative study of elasto-mechanical, electronic and optical properties of pyrochlores. These structures are first optimized and second order-independent cubic elastic constants C11, C12 and C44 are computed using the optimized data. These computed cubic elastic constants are further used to check the mechanical stability, [Poisson's ratio](https://www.sciencedirect.com/topics/materials-science/poisson-ratio), Pugh's ratio and Cauchy pressure which depicts the flexible and ductile nature of both materials. Kleinman ratio is more significant for La2Zr2O7, so it has excellent bond stretching minimization phenomena. [Young's modulus](https://www.sciencedirect.com/topics/materials-science/youngs-modulus) and lame's constants describe that Nd2Zr2O7 is stiffer and difficult to compress than La2Zr2O7. Debye temperature and sound velocities are also calculated for both oxides. Due to the high melting temperature, Nd2Zr2O7 is suitable for high-temperature environments and is used in aerospace and construction industries. Band structures reveal that these oxides are metallic as there appears no gap in electronic dispersion relations. Analysis of the density of states reveals the magnetic nature of these oxides as the density of states is not the perfect image of each other in both spin channels. The imaginary part of the [dielectric](https://www.sciencedirect.com/topics/materials-science/dielectric-material) function also shows the optically metallic nature and suitability for sensors and opto-electronic devices.