# Classification of Oxide Compounds through Data-Mining Density of States Spectra

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**Abstract :**

Pattern recognition techniques were used to extract features from the density of states (DOS) curves derived from density functional theory calculations of over a dozen related oxide systems. Features in the DOS profiles that were associated with crystal structure, chemistry, and stoichiometry were identified. Classification maps identifying trends in the electronic structure with respect to crystal chemistry were created using multivariate analysis methods. It was found that crystal structure appeared to have a more significant impact on the DOS than chemistry for the systems studied. The differences in the electronic structure of HfO2 and ZrO2 were captured as a function of crystal structure, and the features of the DOS curve, which represent these differences, were identified. Correlations between crystal symmetry and metal/oxygen ratio were also uncovered from this type of analysis.

**Journal title / Revue :** Journal of the American Ceramic Society, ISSN : 0002-7820, DOI: 10.1111/j.1551-2916.2011.04476.x, Issue : 9, Volume : 94, pp. 2974- 2980 , SEP 2011.