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Playing dice with Mo-V-Te-Nb oxide ...

… a promising catalyst for alkane oxidation with a structure obscured by the fractional distribution of V or Mo atoms on many sites. In their Communication on page 12854 ff., P. Sautet et al. present an efficient DFT approach that allows fast comparison of the energies of up to 8008 configurations of this complex oxide. The calculations predict the statistical V atom distribution found experimentally, when the dice are loaded and the V/Mo distribution is far from being equiprobable.

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