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Computational identification of a new form of Li2MnSiO4 for battery applications[1] MAXIM ARSENTEV, MARINA KALININA, Institute of Silicate Chemistry of Russian Academy of Sciences — The BMW laboratory identified 12 cathode materials, which offer concrete chances of being used in electric vehicles applications. Amongst them Li2MnSiO4 offer some advantages like high theoretical capacities, environmental friendliness, thermal stability, and inexpensiveness. But Li2MnSiO4 easily undergoes amorphization and shows a poor cyclability due to layer exfoliation and/or need for octahedral coordination for Mn. In this presentation we analyzed the properties of 132 structures of the lithium manganese silicate compounds provided by Materials Project, a core program of the Materials Genome Initiative, to meet the requirements imposed on the cathode material in the long term for 2025. The main selection criteria were stability, specific gravimetric and volumetric capacity, and presence of channels for Li ion migration. Among the 14 selected compounds, only cubic Li2MnSiO4 (P213, space group number 198) was found to have stable analogue – Na2CaSiO4 with the same structure. Using this information, we present the results of the structure stabilization obtained using the ABINIT software.

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