T-Atom Vacancy Formation in Zeolite with Mse Topology

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Following our previous experience in modeling T-atom defects formation in ITQ-44 zeolite framework [1]. We have performed a computational study on the T-atom defect formation in the zeolite with MSE topology. It has been reported that such zeolites with Ti in the framework perform very well in the process of selective phenol oxidation [2]. The role of the Si-vacancy and Ti distribution in the framework was not clarified yet. For this reason, we have performed computational study on this material. The relative energy for the formation of Si-vacancy and substitution of Si for Ti and Al has been studied by means of density functional theory. For all non- equivalent T cites, we have calculated the relative energy for Si vacancy formation. We have found that the easiest Si vacancy can be formed in T8 followed by T3 position, while the formation of Si vacancy in T1, T2, T4 and T5 is thermodynamically unfavorable. The substitution of Si for Ti or Al was also studied. It has been found that Si will be substituted by Ti in T8, T3 and T7 positions in the MSE framework.