**Scientific Achievement**

The industrially-relevant separation of ethylene and ethane was studied computationally: two models, TraPPE-UA and newly developed TraPPE-UA2, were utilized to screen the database of the International Zeolite Association (IZA) for the ability of zeolites to carry out these separations.

**Significance and Impact**

Promising all-silica zeolite structures for adsorptive separation of ethane and ethylene were identified; transport may play a significant role in affecting the performance of these materials.

**Research Details**

TraPPE-UA and TraPPE-UA2 were used to study ethylene and ethane separations in zeolites. A detailed analysis, with regards to accessibility of favorable sites and sensitivity to molecular models was carried out on the top-performing structures.

- DFT, ACO, AWO, UEI, APD, and SBN frameworks are predicted to be selective towards ethylene. Similarly, all-silica NAT and JRY frameworks will be interesting synthesis targets for developing ethane-selective materials.

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Work was performed at University of Minnesota.