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Predictive modeling of surface morphology of multicomponent catalysts for their optimum performance ALTAF KARIM, SYED ISLAMUDDIN SHAH, COMSATS Institute of Information Technology, Islamabad, Pakistan — Multi-component microstructures of artificially engineered catalysts are promising for the best ever performance in alternative fuel production. We have designed and implemented a set of intelligent algorithms capable of predicting the surface morphology of multicomponent catalysts for their optimum performance. For example we come up with three kinds of different catalysts. Based on a database obtained from the density functional theory based kinetic Monte Carlo simulations, the first kind of single component catalytic surface promotes and helps dissociative adsorption of chemical species, but it hinders the diffusion of intermediate species. On the other hand, the second kind of single component catalytic surface promotes the diffusion of intermediate species, but suppresses the reactions and desorption processes. However the third kind of single component catalytic surfaces can significantly enhance reactions among intermediate species. Therefore no single component material surface would be a suitable candidate for becoming a good catalyst. However a combination of all above mentioned kind of materials may exhibit the maximum ever performance. Our algorithm models the surface morphology of these multicomponent catalysts by varying the surface area of each component and also by changing the shape of each component in such a way that the catalyst gives the highest rate of chemical formation. Our results confirm the best ever performance of our artificially engineered catalysts.

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