
icc20
بیستمین کنگره شیمی ایران
17-19 July 2018
Ferdowsi University
Of Mashhad
دانشگاه فردوسی مشهد
انجمن شیمی ایران
Iranian Chemical Society
20th Iranian Chemistry Congress
Certificate
of oral presentation
This document certifies that:
Yalda Sabahi
Presented a paper entitled:
Molecular dynamics as a tool to study effect
of Na^+ cations on diffusion of SO_2 in Y zeolite
Yalda Sabahi, Fatemeh Moosavi
At the 20th Iranian Chemistry Congress(ICC20),
which was held at the Ferdowsi University Of Mashhad, Mashhad, Iran from 17-19 July 2018.
prof. Hossein Eshghi
Conference Chairman
بیستمین کنگره شیمی ایران
prof. Mohammad Ali Zolfigol
Iranian Chemical Society Chairman

Paper code: 120

Molecular dynamics as a tool to study effect of Na^+ cations on diffusion of SO_2 in Y zeolite

Yalda Sabahi[1], Fatemeh Moosavi[*]

Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran

Email: moosavibaigi@um.ac.ir

Since most carbonaceous or hydrocarbon fuels and the ores of many metals contain sulfidic sulfur, as a result, vast volumes are produced in the processing and utilization of hydrocarbon fuels such as power plants, refineries and metallurgical units of metal extraction. High levels of sulfur dioxide production releasing it into the atmosphere is one of the chemical threats to the environment. On the other hand, sulfur dioxide has widespread uses in the wood pulp industry and the manufacture of paper, textile and food processing. However, the outstanding use (more than 98%) is the production of sulfuric acid [1]. The existence of these mutual characteristics has led to the development of adsorption and removal processes. The present study evaluates the diffusion of SO_2 gas in silica Y zeolite cages (Si/Al=∞) and Y zeolite with 48 or 64 Na^+ cations per unit cell (Si/Al=3,2) by MD simulation. All simulations have been done using DL_POLY_2.17 [2] program. The MD simulations were performed within the NVE ensemble at 300, 400, 500 and 600 K. The behavior of SO_2 was investigated for loading of 24 molecules per unit cell **(**mol/u.c.). Self-diffusion coefficients of guest molecules in Y zeolite are presented in Table 1.

Table 1. The computed self-diffusion coefficients, D in 10^{-9} m^2. s^{-1} of SO_2 in Y zeolite, at different temperatures and loading 24 mol/u.c.

T(K)	Silica Y	Si/Al=3	Si/Al=2
300	6.92	0.69	0.75
400	9.38	1.62	2.93
500	13.57	5.78	6.15
600	13.61	7.83	8.23

As the temperature increases, the self-diffusion coefficient increases in all three types Y zeolite, because molecular movements at higher temperatures lead to more successful jump between sites. The presence of Na^+ cations in two zeolites Si/Al=2,3 will lead to a decrease in the diffusion of SO_2. The SO_2 molecules preferentially reside near the cations due to the stronger attraction [3].

References

[1] H. Muller, Sulfur Dioxide. Ullmann's Encyclopedia of Industrial Chemistry, Wiley VCH Verlag GmbH &Co. KgaA, **2000**.

[2] W. Smith, T.R. Forester, Journal of molecular graphics & modelling, **1996**, 14, 136-141.

[3] D. Newsome, M. O. Coppens, Chemical Engineering Science, **2015**, 121, 300-312.