

## **Molecular dynamics simulation of migration fractionation effect of alkylated carbazoles in limestone reservoirs and its application in the Tarim Basin, NW China**

QIUYA HAN<sup>1</sup> MEIJUN LI<sup>1,\*</sup> XIAOQIANG LIU<sup>1,2</sup>  
ZICHENG CAO<sup>3</sup>

<sup>1</sup> State Key Laboratory of Petroleum Resources and Prospecting, College of Geosciences, China University of Petroleum, Beijing 102249, China

(\*correspondence: meijunli@cup.edu.cn)

<sup>2</sup> College of Chemistry and Environmental Engineering, Sichuan University of Science and Engineering, Zigong 643000, China

<sup>3</sup> Exploration and Development Research Institute, Northwest Oilfield Branch Corporation, SINOPEC, Urumqi 830011, Xinjiang, China

Carbazole (CA) and its methyl and dimethyl substituted homologues are the common nitrogen-containing polycyclic aromatic compounds in crude oils. The ratio of 4-/1-methylcarbazole and 2,5-/1,8-dimethylcarbazole have been substantially applicable in sandstone reservoirs to trace oil migration orientation and pathways. In this study, we focus on geo-chromatographic fractionation effect of aforementioned alkylcarbazoles in limestone reservoir. As a practical and effective method, the molecular dynamic (MD) simulation have been successful applied in petroleum organic geochemistry, such as the migration fractionation effect of dibenzofurans. Here we calculated the energy of interaction between some alkylcarbazoles and calcite surface using MD simulation. The results show that 4-methylcarbazole (4-MCA) and 2,5-dimethylcarbazole (2,5-DMCA) have a slight preference for being adsorbed on calcite surface over 1-methylcarbazole (1-MCA) and 1,8-dimethylcarbazole (1,8-DMCA), respectively. In addition, we calculated the solubility of these alkylcarbazoles, which indicates the molecules more easily adsorbed on the calcite surface are less soluble in water. It just right suggests that for the oil-wet reservoir the ratio of 4-/1-MCA and 2,5-/1,8-DMCA decrease with increasing migration distance. It is further shown in theory that migration fractionation mechanism of some alkylated carbazole isomers in limestone reservoir at the molecular level. These two indicators were also applied successfully in Ordovician carbonate reservoir in the Tuoputai region, Tarim Basin, NW China and can be used as effective molecular markers for tracing migration orientation and pathways.