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Silica nanopores as nanocontainers for cisplatin: Molecular dynamics study of a targeted drug delivery system

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The diffusion and adsorption behavior of cisplatin in silica nanopores is investigated using molecular dynamics simulation. Two different silica conformations are studied in order to characterize the influence of surface polarity. We find a strong influence of the pore diameter on the diffusion coefficient; only for pore diameters larger than roughly 1.6 nm, cisplatin assumes the same diffusion coefficient as in bulk water. Our results also allow estimating escape times of cisplatin from a pore. Acceleration techniques are used in order to sample adsorption phase space efficiently and to identify realistic adsorption conformations. We find major differences between the polar and nonpolar surfaces. Electrostatic interactions govern the adsorption on polar surfaces and can be described by the alignment of the molecule dipole with the surface dipole; hence, spreading of the molecule on the surface is irrelevant. On nonpolar surfaces, on the other hand, van-der-Waals interaction dominates inducing surface spreading of the molecule.

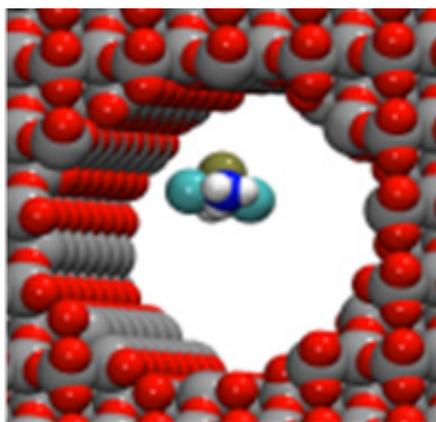


Figure : Momentary configuration of cisplatin in the axial R=10 Å pore at time 488 ps.

Recent Publications

1. Oliveira L, et al. (2016) Functionalized silica nanoparticles: an alternative platform for targeted drug delivery of water insoluble drugs. *Langmuir* 32:3217–3225.
2. Panczyk T, et al. (2013) Molecular dynamics study of cisplatin release from carbon nanotubes capped by magnetic nanoparticles. *Journal of Physical Chemistry* 117 (33):17327–17336.
3. J M Rimsza and Jincheng Du (2013) Structural and mechanical properties of nanoporous silica. *J. Am. Ceram. Soc.* 97(3):772–781.
4. Shahbazi M, et al. (2012) Nanostructured porous Si-based nanoparticles for targeted drug delivery. *Biomatter*. 2(4):296–312.
5. Haiary S, et al. (2012) Nanoporous silicon as drug delivery systems for cancer therapies. *Journal of Nanomaterials* p15

Biography

Marjan A Nejad is a PhD candidate in Kaiserslautern University in Germany. She is doing her research in Molecular Dynamic Studies in Drug Delivery System..

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