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Appendix

A. Alternative scaling parameters

In this Appendix, two alternative definitions for the scaling parameter θ are discussed in order to further support the one discussed in the main text. The first alternative definition is based on the notion of interfacial work; while the second one makes an attempt to incorporate also the water density / hydration level.

Inspired by other successful works, where a scaling behavior could be found by resorting to the notion of interfacial work [327, 599], the first attempt in searching for the scaling parameter was focused on the following argument. Let us consider the schematics in Figure 2.19c. Inspired by the computation of $\delta^{(p)}$ for an arbitrary particle p, a characteristic energy $\varepsilon^{(p)}$ can be defined as:

$$\varepsilon^{(p)} = \frac{\sum_{i=1}^{N_a} \varepsilon_i^{(p)} S_{loc,i}}{S_{tot}}, \tag{A.1}$$

where $\varepsilon_i^{(p)}$ represents the well depth of the potential energy shown in Figure 2.19b. Since the interfacial work between a particle and the solvent is proportional to the above $\varepsilon^{(p)}$, a possible guess for the scaling quantity would be:

$$\theta_e = \frac{1}{V_w} \frac{\sum_p \varepsilon^{(p)} V_{in}^{(p)}}{N_A k_B T}, \tag{A.2}$$

where N_A and $V_{in}^{(p)}$ are the Avogadro Number and the volume of influence of particle p, respectively. However, if θ_e is assumed as a unique independent variable for scaling the D values, a poor correlation appears, as evident in Figure A.1. Hence, θ_e was judged not suitable for the scaling purpose.

Second, the suggested scaling parameter θ in Equation 2.16 does not include the density of water within the analyzed configurations. In fact, the considered MD setups are characterized by a range of hydration levels (from 660 to 1080 kg m^{-3}) where no heterogeneous wetting or anomalous behavior due to low water filling regimes are expected [92, 161]. Towards

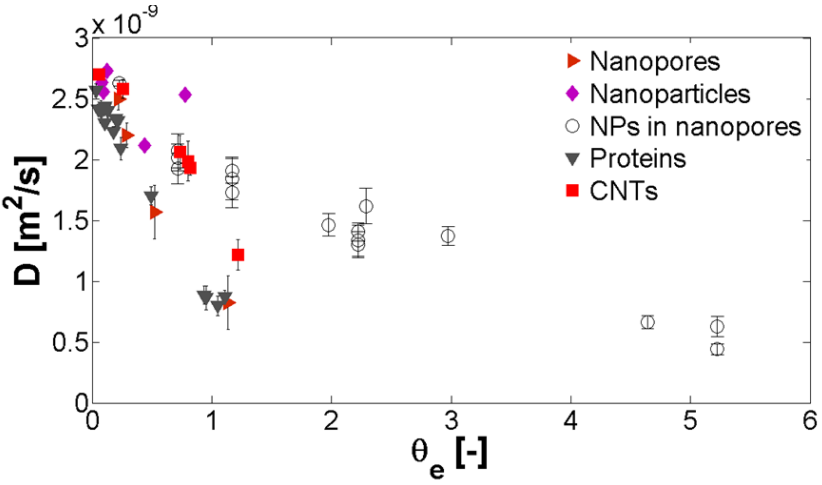

Figure A.1.: Alternative dimensionless parameter θ_e. D self-diffusion coefficient of water vs. the dimensionless parameter θ_e based on the interfacial work. For simplicity, only a subset of the analyzed cases are reported.

an effort of incorporating also the hydration level, the following variable θ_d can be also considered as a scaling parameter:

$$\theta_d = \frac{\rho_B}{\rho}\theta, \tag{A.3}$$

where ρ_B is the bulk density of water (given the pressure and the temperature), ρ is the actual water density in the setup, while θ is the suggested scaling variable previously defined by Equation 2.16. In Figure A.2 and 2.21 are reported the results obtained when the scaling variables θ_d and θ are used, respectively.

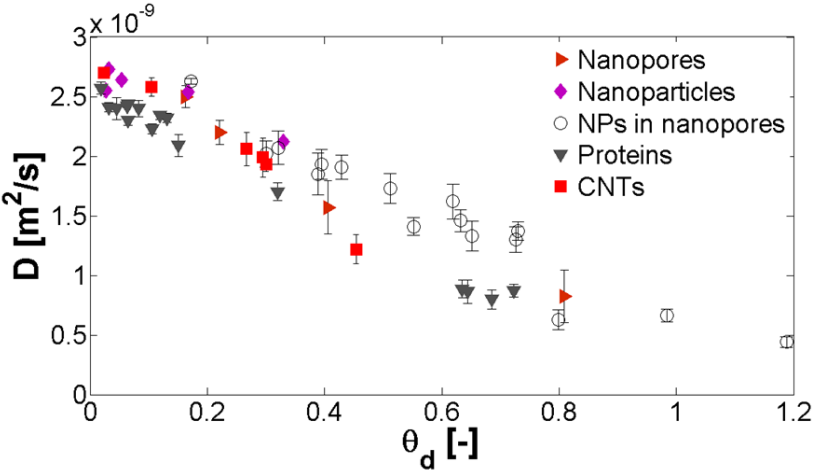

Figure A.2.: Alternative dimensionless parameter θ_d. D self-diffusion coefficient of water vs. the dimensionless parameter θ_d, which also takes into account the density of water of the system. For simplicity, only a subset of the analyzed cases are reported.

B. Detailed Molecular Dynamics results

In this Appendix, the detailed list of molecular dynamics configurations and results discussed in Chapter 2 and 6 are reported.

In Table B.1, D is evaluated according to different diameters of silica nanopores; in Table B.4, the D obtained around silica or magnetite NPs at different concentrations (i.e. L size of the water box) is shown; in Tables B.2 and B.3, different configurations of nanopores filled by NPs are simulated. In Table B.5, the effect of water density on D is explored; whereas in Tables B.6, B.7 and B.8 the effects of forcefield (i.e. strength of attractive nonbonded forces on solid surface) are evaluated. In Tables B.9 and B.10, the D obtained around CNTs or proteins at different concentrations (i.e. L size of the water box) are shown, respectively. In Table B.11, D of bulk water is computed. Notice that, in Case 10 and Case 12, NPs are initially placed randomly within the silica nanopore, whereas in all other cases NPs are initially placed on the surface of silica nanopore, where they tend to adsorb during the remaining time of computation.

Finally, Table B.12 details the simulated configurations of Gd(DOTA) either bonded to silica wall or in bulk water.

Case	Φ [nm]	ϕ [nm]	N	ρ [kg m^{-3}]	T [K]	Charges	ε_{Fe} [kJ/mol]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
1	2.03	-	0	818	300	Default	-	0.367	**0.663**	**8.24E-10**	2.20E-10
2	4.05	-	0	903	300	Default	-	0.333	**0.366**	**1.57E-09**	2.22E-10
3	8.13	-	0	913	300	Default	-	0.331	**0.202**	**2.20E-09**	1.01E-10
4	11.04	-	0	923	300	Default	-	0.329	**0.150**	**2.50E-09**	8.98E-11

Table B.1.: MD simulations and results for silica nanopores with different diameters Φ.

Case	Φ [nm]	ϕ [nm]	N	ρ [kg m^{-3}]	T [K]	Charges	ε_{Fe} [kJ/mol]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
5	8.13	1.97	2	859	300	Default	24.94	S:0.331/M:0.497	**0.276**	**2.07E-09**	1.41E-10
6	8.13	1.97	4	838	300	Default	24.94	S:0.331/M:0.497	**0.360**	**1.91E-09**	1.01E-10
7	8.13	1.97	8	797	300	Default	24.94	S:0.331/M:0.497	**0.519**	**1.33E-09**	1.27E-10
8	8.13	1.97	16	663	300	Default	24.94	S:0.331/M:0.497	**0.787**	**4.41E-10**	4.49E-11

Table B.2.: MD simulations and results for silica nanopores ($\Phi = 8.1$ nm) filled by a varying number N of magnetite NPs ($\phi = 2.0$ nm). Note that 'S' stands for silica nanopores, while 'M' for magnetite nanoparticles.

Case	Φ [nm]	ϕ [nm]	N	ρ [kg m^{-3}]	T [K]	Charges	ε_{Fe} [kJ/mol]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
9	8.13	1.27	16	812	300	Default	24.94	S:0.331/M:0.461	**0.513**	**1.46E-09**	9.15E-11
10	11.04	1.27	36	873	300	Default	24.94	S:0.329/M:0.461	**0.540**	**1.62E-09**	1.46E-10
11	11.04	1.97	20	808	300	Default	24.94	S:0.329/M:0.497	**0.590**	**1.37E-09**	7.79E-11
12	11.04	1.27	66	786	300	Default	24.94	S:0.329/M:0.461	**0.774**	**6.63E-10**	5.14E-11

Table B.3.: MD simulations and results for silica nanopores with diameter Φ filled by N magnetite NPs with diameter ϕ. Note that 'S' stands for silica nanopores, while 'M' for magnetite nanoparticles.

Case	Mat.	ϕ [nm]	L [nm]	N	ρ [kg m^{-3}]	T [K]	Charges	ε_{Fe} [kJ/mol]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
13	SiO_2	5.22	6	1	935	300	Default	-	0.327	**0.309**	**2.12E-09**	3.78E-11
14	Fe_3O_4	5.22	8	1	974	300	Default	24.94	0.533	**0.164**	**2.53E-09**	3.54E-11
15	SiO_2	5.22	7	1	926	300	Default	-	0.327	**0.159**	**2.63E-09**	2.32E-11
16	Fe_3O_4	1.97	7	1	991	300	Default	24.94	0.461	**0.032**	**2.73E-09**	4.93E-11
17	Fe_3O_4	1.27	6	1	988	300	Default	24.94	0.497	**0.027**	**2.55E-09**	5.32E-11

Table B.4.: MD simulations and results for a silica or magnetite NP with diameter ϕ, immersed in a cubic box of water with edge L.

Case	Φ [nm]	ϕ [nm]	N	ρ [kg m^{-3}]	T [K]	Charges	ε_{Fe} [kJ/mol]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
18	8.13	1.97	2	919	300	Default	24.94	S:0.331/M:0.497	**0.276**	**2.02E-09**	1.09E-10
19	8.13	1.97	4	925	300	Default	24.94	S:0.331/M:0.497	**0.360**	**1.85E-09**	1.75E-10
20	8.13	1.97	8	941	300	Default	24.94	S:0.331/M:0.497	**0.519**	**1.40E-09**	7.33E-11
21	8.13	1.97	16	985	300	Default	24.94	S:0.331/M:0.497	**0.787**	**6.29E-10**	8.38E-11
22	8.13	1.97	2	698	300	Default	24.94	S:0.331/M:0.497	**0.276**	**1.92E-09**	1.25E-10
23	8.13	1.97	4	702	300	Default	24.94	S:0.331/M:0.497	**0.360**	**1.73E-09**	1.27E-10
24	8.13	1.97	8	715	300	Default	24.94	S:0.331/M:0.497	**0.519**	**1.30E-09**	1.06E-10

Table B.5.: MD simulations and results for silica nanopores (Φ = 8.1 nm) filled by a varying number N of magnetite NPs (ϕ = 2.0 nm), according to different densities of water ρ within the nanopore. Note that 'S' stands for silica nanopores, while 'M' for magnetite nanoparticles.

Case	Φ [nm]	ϕ [nm]	N	ρ [kg m^{-3}]	T [K]	Charges	ε_{Fe} [kJ/mol]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
25	8.13	1.97	2	859	300	Default	2.49	S:0.331/M:0.447	**0.256**	**2.16E-09**	2.25E-10
26	8.13	1.97	2	859	300	Default	12.47	S:0.331/M:0.496	**0.268**	**2.07E-09**	1.46E-10
27	8.13	1.97	4	838	300	Default	2.49	S:0.331/M:0.447	**0.322**	**1.92E-09**	6.64E-11
28	8.13	1.97	4	838	300	Default	12.47	S:0.331/M:0.496	**0.346**	**1.91E-09**	1.12E-10
29	8.13	1.97	8	797	300	Default	2.49	S:0.331/M:0.447	**0.453**	**1.47E-09**	1.09E-10
30	8.13	1.97	8	797	300	Default	12.47	S:0.331/M:0.496	**0.496**	**1.35E-09**	6.45E-11
31	8.13	1.97	16	663	300	Default	2.49	S:0.331/M:0.447	**0.704**	**4.97E-10**	5.78E-11
32	8.13	1.97	16	663	300	Default	12.47	S:0.331/M:0.496	**0.760**	**4.11E-10**	3.48E-11

Table B.6.: MD simulations and results for silica nanopores (Φ = 8.1 nm) filled by a varying number N of magnetite NPs (ϕ = 2.0 nm), according to different values of Lennard-Jones potential of iron atoms ε_{Fe}. Note that 'S' stands for silica nanopores, while 'M' for magnetite nanoparticles.

Case	Φ [nm]	ϕ [nm]	N	ρ [kg m^{-3}]	T [K]	Charges	ε_{Fe} [kJ/mol]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
33	8.13	1.97	8	797	300	S:Default M:Neutral	24.94	S:0.331/M:0.363	**0.519**	**1.64E-09**	4.46E-11
34	8.13	1.97	8	797	300	S:Neutral M:Neutral	24.94	S:0.330/M:0.363	**0.519**	**1.69E-09**	1.98E-10

Table B.7.: MD simulations and results for silica nanopores (Φ = 8.1 nm) filled by 8 magnetite NPs (ϕ = 2.0 nm), according to different values of partial charges of silica or magnetite surfaces. In Case 33, the partial charges on magnetite surface are set to zero; in Case 34 all the partial charges of the setup are set to zero.

Case	Mat.	ϕ [nm]	L [nm]	N	ρ [kg m^{-3}]	T [K]	Charges	ε_{Fe} [kJ/mol]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
35	SiO_2	1.97	5	1	990	300	Fe_3O_4 partial charges on SiO_2	-	0.326	**0.054**	**2.64E-09**	3.11E-11

Table B.8.: MD simulations and results for a silica NP ($\phi = 2.0$ nm) in a cubic box of water ($L = 5.0$ nm). Partial charges of silanol groups are modified according to the magnetite force-field, namely $q_{SI(H)} = 1.21$ e, $q_{O(H)} = -1.61$ e and $q_H = 0.40$ e.

Case	Chirality	Φ [nm]	L [nm]	V [nm^3]	ρ [kg m^{-3}]	T [K]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
36	(5,5)	0.68	4.8	21.1	1076	300	0.286	**0.489**	**1.22E-09**	1.24E-10
37	(5,5)	0.68	4.8	73.6	989	300	0.286	**0.104**	**2.58E-09**	7.89E-11
38	(5,5)	0.68	4.8	315.6	971	300	0.286	**0.022**	**2.70E-09**	4.36E-11
39	(10,10)	1.4	9.8	131.9	989	300	0.368	**0.291**	**1.99E-09**	1.64E-10
40	(20,20)	2.7	9.8	260.1	989	300	0.369	**0.296**	**1.93E-09**	5.89E-11
41	(30,30)	4.1	9.8	431.4	989	300	0.369	**0.264**	**2.06E-09**	1.39E-10

Table B.9.: MD simulations and results for carbon nanotubes (Φ diameter, L length) solvated in triclinic water boxes with V volumes.

Case	Protein	SAS [nm^2]	V [nm^3]	ρ [kg m^{-3}]	T [K]	δ [nm]	θ [nm]	D [m^2 s^{-1}]	+/-
42	B1 Immunoglobulin	36.4	23.1	934	300	0.295	**0.675**	**8.72E-10**	5.22E-11
43	B1 Immunoglobulin	36.4	24.0	934	300	0.295	**0.639**	**7.98E-10**	8.01E-11
44	B1 Immunoglobulin	36.4	25.7	903	300	0.295	**0.582**	**8.64E-10**	9.98E-11
45	B1 Immunoglobulin	36.4	26.0	899	300	0.295	**0.571**	**8.85E-10**	7.40E-11
46	B1 Immunoglobulin	36.4	347.5	989	300	0.295	**0.032**	**2.41E-09**	3.80E-11
47	Ubiquitin	48.2	60.0	936	300	0.309	**0.300**	**1.70E-09**	7.42E-11
48	Ubiquitin	48.2	111.8	976	300	0.309	**0.147**	**2.09E-09**	9.13E-11
49	Ubiquitin	48.2	252.2	979	300	0.309	**0.062**	**2.42E-09**	1.35E-11
50	Ubiquitin	48.2	347.5	989	300	0.309	**0.044**	**2.39E-09**	9.31E-11
51	Ubiquitin	48.2	816.6	993	300	0.309	**0.019**	**2.57E-09**	5.14E-11
52	Green Fluorescence Protein	108.8	347.5	989	300	0.302	**0.105**	**2.23E-09**	4.06E-11
53	Ca^{2+}-ATPase	448.2	1214.8	989	300	0.309	**0.129**	**2.32E-09**	3.93E-11
54	Glucokinase	198.2	579.9	989	300	0.302	**0.117**	**2.34E-09**	3.20E-11
55	Leptin	68.9	347.4	989	300	0.306	**0.064**	**2.44E-09**	1.73E-11
56	Myoglobin	90.7	347.4	989	300	0.295	**0.082**	**2.40E-09**	6.84E-11
57	Lysozyme	67.4	347.4	989	300	0.315	**0.065**	**2.30E-09**	3.86E-11

Table B.10.: MD simulations and results for proteins, with SAS surface accessible surface, solvated in water boxes with Vvolumes.

Case	Mat.	L [nm]	ρ [kg m^{-3}]	T [K]	θ [nm]	D [m^2 s^{-1}]	+/-
58	Water	1.9	1004	300	**0**	**2.60E-9**	6.26E-11

Table B.11.: MD simulations and results for SPC/E water in a cubic box of water (L = 1.9 nm).

Gd(DOTA) bonded to silica wall

Case	b [nm]	d_{min} [nm]	τ_E [ps]	$\tau_E/\tau_{R,bulk}$ [-]	S^2 [-]	R^2 [-]	T [ns]	Δt [ns]	M [-]	N [-]
1	0.4	0.21	46.2	0.62	0.86	0.84	3.5	2	4	2
2	0.5	0.23	34.6	0.46	0.86	0.85	3.5	2	4	2
3	0.8	0.26	210.5	2.81	0.26	0.94	10	8	3	2
4	1	0.51	149.4	1.99	0.05	0.96	7	4	4	2
5	1	0.36	172.3	2.30	0.06	0.97	7	4	4	2
6	2	1.29	90.3	1.20	0.03	0.99	3.5	2	4	2
7	3	2.00	74.0	0.99	0.02	0.98	3.5	2	4	2

Gd(DOTA) in bulk water

Case	b [nm]	d_{min} [nm]	$\tau_{R,bulk}$ [ps]	S^2 [-]	R^2 [-]	T [ns]	Δt [ns]	M [-]	N [-]
8	-	-	75.0 (300 K)	0.00	0.98	3.5	2	4	2
Exp	-	-	77±4 (298 K)	-	-	-	-	-	-

Table B.12.: Details of the simulated Gd(DOTA) and/or silica wall setups by means of molecular dynamics simulations. Experimental τ_R of Gd(DOTA) immersed in bulk water is taken from Reference [579]. d_{min} is evaluated as the mean minimum normal distance between silica wall and Gd(DOTA) atoms during the simulated trajectory, whereas $d = d_{min} + r_{Gd(DOTA)}$, where $r_{Gd(DOTA)} \cong 0.5$nm (see Figure 6.6). Note that R^2 is the coefficient of determination of the Lipari-Szapo fitting, T is the simulation time, Δt is the time span of the RACFs; M is the amount of RACFs evaluated per trajectory; N is the number of trajectories analyzed for the same setup (i.e. repetitions), with random initial velocities. For example, in Case 1 RACFs are calculated in the intervals 0–2 ns, 0.5–2.5 ns, 1–3 ns and 1.5–3.5 ns on the two trajectories available.

C. WANA software

In this Appendix, a software for the automatic evaluation of the characteristic length of nanoconfinement δ of a solid surface is presented. The software is named "WAter NAnoconfinement evaluation package" (WANA), and it allows to calculate δ thus θ (Equation 2.16) once the water nanoconfinement conditions (i.e. geometry and surface potential of the solid interfaces) are known. Self-diffusivity of water can be then computed by the scaling law in Equation 2.20.

First, the purposes and architecture of the software are described; then a brief tutorial of the WANA functioning is detailed. Note that the first release of WANA software can be readily downloaded from `http://areeweb.polito.it/ricerca/small/nano/wana/`, whereas a more complete version will be soon presented in a detailed scientific article and shared in a open-access library.

Purposes and architecture

An accurate prediction of self-diffusivity of water under nanoconfined conditions is fundamental in a broad variety of technologies and biological processes. For example, water adsorption or infiltration in nanoporous materials are exploited for sieving, thermal storage or desalination devices (Chapters 4 and 5), whereas the reduction of water mobility in the proximity of solid surfaces is essential for the rational design of nanoparticles for biomedical applications (Chapter 6). Atomistic simulations and theoretical considerations have been widely studied for better understanding the water diffusion properties under nanoconfined conditions (Chapter 2). However, a gap between modeling knowledge and technological exploiting of the water nanoconfined properties still exist. In this context, WANA software is realized with the specific aim to make more accessible the estimation of water self-diffusivity under nanoconfined conditions to non-specialists, such as manufacture engineers, biologists or physicians.

WANA software allows to compute the characteristic length of nanoconfinement δ and the mean attractive potential well of solid-liquid nonbonded interactions from the numerical results obtained by simple preprocessing tools (e.g. energy minimization algorithms) available in GROMACS package [27]. Therefore, the need to run a full and computationally intensive molecular dynamics simulation is no more required for determining water properties under nanoconfined conditions, such as within nanopores, around nanoparticles, carbon nanotubes or biological molecules.

The software is implemented as a MATLAB® script, in order to allow the modification and further development of the code by experts. Moreover, the package is accompanied by a Graphical User Interface (GUI), which is designed for simplifying the basic usage of the software by nonspecialists.

Running WANA requires:

- A coordinate file (e.g. **.pdb*) describing the structure of interest (e.g. nanopores, nanoparticles, carbon nanotubes or biological molecules);
- GROMACS (`http://www.gromacs.org`, version 4.5.7 or above) software, which is an open-access molecular dynamics engine. Note that any other software able to generate the Solvent Accessible Surface (SAS) of a given geometry could be analogously adopted;
- MATLAB® R2009b (`http://www.mathworks.com`) software. Note that older releases of the software have been successfully tested for compatibility;
- A nearest neighbors routine. In particular, such a routine should be able to locate the nearest neighbors (according to Euclidean distance) within a fixed radius as well as the k nearest neighbors to a given point (for a fixed integer k). To this purpose, the open source script *nearestneighbour.m* by Richard Brown is suggested, which is freely downloadable at Matlab Central website (`http://www.mathworks.it/matlabcentral/fileexchange/12574-nearestneighbour-m`). Obviously, at the user option, any other routine for the search of nearest neighbor can be utilized instead;
- A table with an estimate of the relative permittivity of water as a function of distance from the charged surface. In the current WANA release, data are taken from Reference [176];
- WANA software.

Software tutorial

Given a certain geometrical configuration, where water molecules are nanoconfined, and by referring to the flow-chart in Figure C.1, the main steps involved in the computation of the scaling parameter θ are reported. For the sake of completeness and without loss of generality, a few GROMACS commands are also given as example. The described procedure can be properly rearranged by a well educated user of other MD software packages.

First, input files for WANA software have to be prepared:

1. Download or generate the dry geometry of interest (i.e. **.pdb* file). Large databases of nanoscale geometries are available in the Web, for example the Protein Data Bank (`http://www.rcsb.org`) for biological molecules, the PubChem Project (`https://pubchem.ncbi.nlm.nih.gov/`) for chemical compound or the ZEOMICS Project for microporous materials (`http://helios.princeton.edu/zeomics/`);

2. Chose a suitable force field for the solid-liquid nonbonded interactions, in the form of 12-6 Lennard Jones and/or Coulomb potentials. The latter can be either user-defined or extracted from the libraries of molecular dynamics software (e.g. GROMOS, AMBER, CHARMM, ...);

3. Create a topology file containing the coordinates of the atoms of the confining surface and their force field parameters;

   pdb2gmx -f geometry.pdb -o geometry_0.gro -p topology.top -i restraints.itp -water spce

   editconf -f geometry_0.gro -o geometry.gro -bt triclinic -d 2 -c

   or

   editconf -f geometry.pdb -o geometry.gro -bt triclinic -d 2 -c

   g_x2top -f geometry.gro -o topology.top -ff forcefield -noparam -pbc

4. Perform energy minimization of the particle in vacuum (not necessary if the initial geometry is the equilibrium configuration of the molecule);

   grompp -f em.mdp -c geometry.gro -p topology.top -o em.tpr

   mdrun -s em.tpr -o trajectory.trr -c geometry-em.gro -e em.edr

5. Solvate the system by a proper water model (e.g. SPCE, TIP3P, TIP4P, ...);

   genbox -cp geometry-em.gro -cs spc216.gro -o geometry_sol.gro -p topology.top

6. Perform energy minimization of the solvated setup;

   grompp -f em_sol.mdp -c geometry_sol.gro -p topology.top -o em_sol.tpr

   mdrun -s em_sol.tpr -o trajectory_sol.trr -c geometry_sol-em.gro -e em_sol.edr

7. Use the output trajectories from step 6 to obtain the Connolly surface (in the form of a geometry **.pdb* file) [173], the local and the total SAS (**.xvg* file) of the confining solid surface. To this purpose, *g_sas* is the most adapt post-processing function readily available in GROMACS.

   g_sas -f trajectory_sol.trr -s em_sol.tpr -o sas.xvg -oa atom_sas.xvg -q connolly.pdb

At this point, four files are obtained, namely:

1. *topology.top*, topology file describing the structure of interest;
2. *itpfile.itp*, database of the nonbonded 12-6 Lennard-Jones and/or Coulomb interactions between the atoms of the considered geometry;
3. *atom_sas.xvg*, text file containing the SAS per atom of the solid surface;
4. *connolly.pdb*, coordinates of the Connolly surface for the molecule.

The latter files have to be grouped in a folder, which will be the input source for the WANA software.

WANA software is then launched by running the Matlab® script *deltasas-gui.m*, which initializes the GUI. Figure C.2 shows the preliminary operations needed for setting up WANA computations, namely: (1) Input the system temperature ([K]), the fraction of kinetic energy to be considered (see Chapter 2 for further details), the cutoff radius to be used for nonbonded interactions ([Å]) and the Lorentz-Berthelot combination rule for Lennard-Jones potentials (1 – arithmetic mean for σ, geometric mean for ε; 2 – geometric mean for both σ and ε); (2) Generate a **.txt* file where the output of WANA computations will be written. The default name of

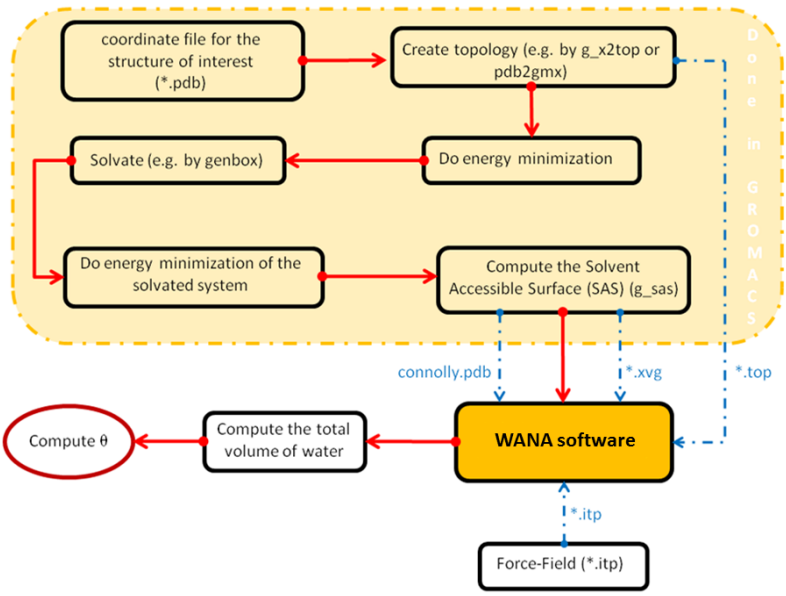

Figure C.1.: Steps leading to the computation of the scaling parameter θ. Red arrows indicate the chronological sequence, while dashed blue lines indicate the provenience of the input files for WANA software. Note that the operations with yellow background are performed by a proper molecular dynamics software (e.g. GROMACS).

the output file is given by the date and time of creation; however, it can be properly renamed by hand.

After that, input files have to be loaded to the WANA environment. Figure C.3 shows the sequence of operations for (1) loading the input folder, which contains the **.pdb*, **.xvg*, **.top* and **.itp* files previously prepared, and (2) start the WANA computation. The obtained results are the characteristic length of nanoconfinement ([nm]), the Solvent Accessible Surface ([nm^2]) and the nonbonded potential well for the confining solid surfaces ([kJ/mol]), and they are shown both in the right-hand side window of the GUI and written to the output **.txt* file.

Finally, once the accessible volume of water (V_w) is estimated following

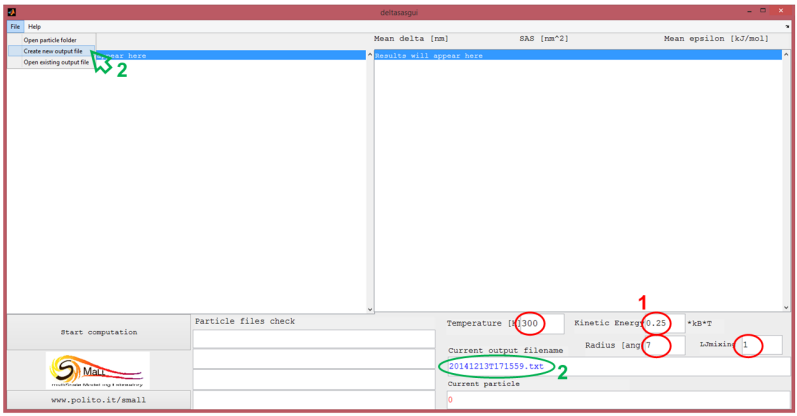

Figure C.2.: Preliminary operations to be performed for computing the characteristic length of nanoconfinement by WANA software.

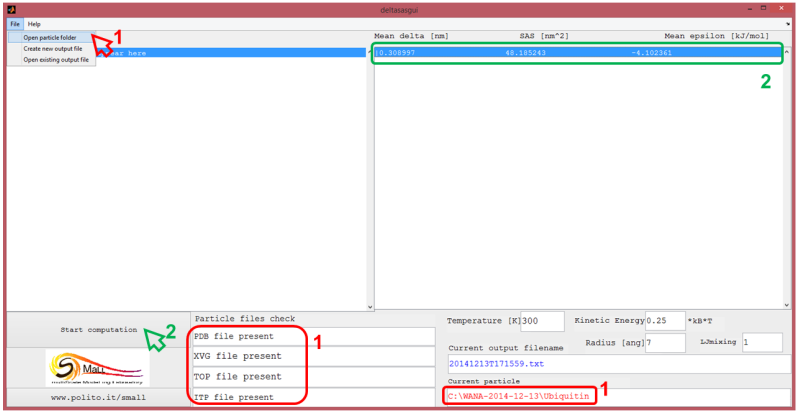

Figure C.3.: WANA computation and outputs, namely the characteristic length of nanoconfinement ([nm]), the Solvent Accessible Surface ([nm^2]) and the nonbonded potential well of the confining solid surfaces ([kJ/mol]).

one of the procedures suggested in Chapter 2, θ parameter can be easily computed from Equation 2.16, whereas the self-diffusivity of water under

such nanoconfined conditions obtained from the scaling law in Equation 2.20.

D. GROTOLAM script

In the last twenty years, numerous molecular dynamics software have been developed to analyze a large variety of microscopic systems. Although they share the same methodology, they have been developed focusing on particular fields of application (e.g. GROMACS for biomolecules; LAMMPS for inorganic compounds) thus implementing specific (but complementary) running and post-processing capabilities. Hence, current open access molecular dynamics software show different structures of the code as well as of the input/output file formats. This led to a microcosm of different languages and standards, which tangles up the researchers interested to use more than one molecular dynamics software for a synergistic usage of the available running and post-processing functionalities. In this confusing framework, the increase of portability between language patterns of different MD software is urgently needed. Despite some isolated and incomplete attempts [600], a simple, modular, robust and consistent solution to the issue is still far from being achieved. In this Appendix, the "GROMACS to LAMMPS" script (GROTOLAM) is presented and its translation accuracy tested.

Structure and functioning

GROTOLAM aims to automatically translate GROMACS input files to LAMMPS ones in a modular way, i.e. allowing to progressively increase both the compatibility between those two software and to add further MD software as export options. GROTOLAM is a MATLAB® code, which will be soon presented in a detailed scientific article and shared in a open-access library. The main script of the package is named *GROTOLAM.m*,

This Section has been developed also thanks to the work of Gianmarco Ciorra for his Master thesis in Mechanical Engineering at Politecnico di Torino. Further details are available in Reference [331].

and it sequentially calls a few sub-functions for converting parts of the system geometry and force field from GROMACS to LAMMPS, in a modular way. The latter sub-functions make the script flexible and able to read different force field types. In the current version, GROTOLAM is able to convert force fields either user-defined or extracted from the GROMACS libraries GROMOS and OPLS, but further extensions will be soon available.

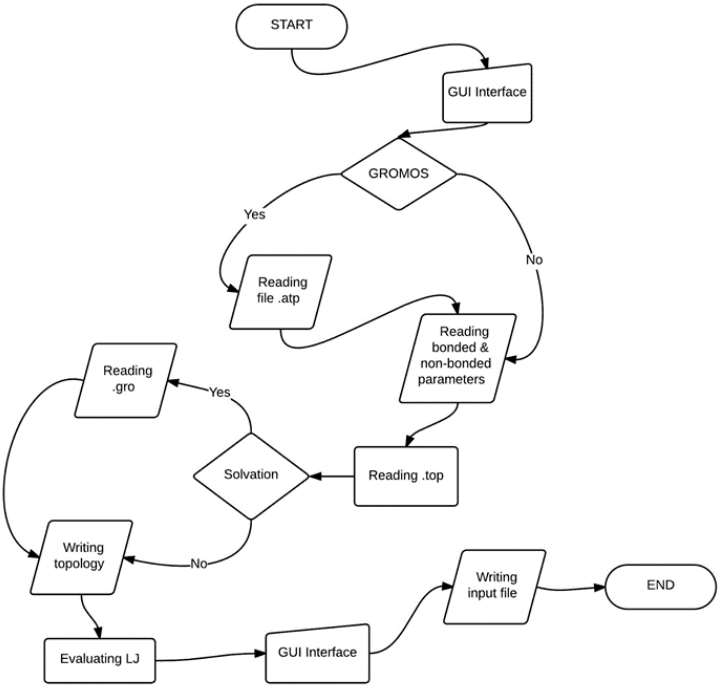

Figure D.1.: Flow chart of the GROTOLAM script.

The algorithm is equipped with two simple Graphical User Interfaces (GUI), which allow to choose how the translation process has to be carried out. In the fist GUI, the user is asked to define the following translation options:

- *Atom Style*. User is asked to choose among *atomic*, *angle* or *full* styles as interaction potentials for the atoms in the configuration

to be translated. *Atomic* style considers only intermolecular non electrostatic interactions (e.g. Lennard Jones or Buckingham potentials); *angle* style adds intramolecular bond and angle potentials to the *atomic* style capabilities; *full* style introduces electrostatic interactions to the *angle* style options.

- *Solvation.* User is asked to define the solvent type in the considered setup. In the current version of GROTOLAM, three points water models (e.g. SPC/E, SPC, TIPS, TIP3P) and sodium ions are compatible with the algorithm.

- *Bond input.* User can choose the input source for the bonded parameters, namely *ITP* if they have to be read from the GROMACS **.itp* file or *TOP* from **.top* file. The latter possibility is useful for user-defined force fields.

- *Force field.* User is asked to select the type of force field to be used, either *GROMOS*, *OPLSA* or *Custom.*

- *Solvent name.* User has to input the name of the group to be considered as solvent in the GROMACS input files.

The second GUI allows to select the statistical ensemble according to which the simulation will be performed, namely NVT, NPT or NVE. The GUI guides users to define the parameters required by the ensemble subroutine, more specifically:

- NVT requires the system equilibrium temperature and the temperature dumping factor;

- NPT requires the system equilibrium temperature and pressure, as well as the temperature and pressure dumping factors and direction of box shrinking;

- NVE directly writes on the LAMMPS input file the *fix nve* command.

Finally, a *DONE* button concludes the definition of the ensembles and starts the final translation.

Translation procedure begins by loading **.top* (topology, which contains partial charges, masses and - possibly - bonded parameters), **.gro* (geometry, which contains atoms coordinates and box size) and **.itp* (force field, which contains both bonded and nonbonded parameters) files in the GROTOLAM environment.

First, force field is imported. Regarding nonbonded interactions, GROTOLAM script automatically recognizes whether Van der Walls interactions are modeled by 12-6 Lennard-Jones potential or by Buckingham one, whereas Coulomb potential is used for partial charges. The Lennard-Jones cross parameters are computed using the Lorentz-Berhelot mixing rule, and the output parameters converted in LAMMPS's *real* units. Regarding bonded interactions, the current version of GROTOLAM is compatible with the following potential types:

- Bond potentials: harmonic, Morse;
- Angle potentials: harmonic, Urey-Bradley;
- Dihedral potentials: proper, Fourier, improper.

If GROMOS force field is selected, the fourth power bond potential from GROMACS is properly converted in an equivalent LAMMPS harmonic bond potential. The latter conversion leads to a discrepancy, but the fourth power bond potential is not yet implemented in LAMMPS thus second power potential is the closest approximation available.

Second, **.top* and **.gro* files are read. Atom types, atom and molecule indexes, charges and coordinates are saved to the GROTOLAM environment. The current version of the algorithm is only compatible with three points water models and sodium ions.

Once all the GROMACS input files are imported, GROTOLAM writes the topology file for LAMMPS. According to the atom style chosen by the user, different geometry data files are produced. These files include all the geometrical information required to run a LAMMPS simulation. Finally, GROTOLAM generates a draft of the LAMMPS input file, which contains commands and physical parameters to carry out the simulation in NVT, NPT or NVE ensemble.

Script benchmark

In this Section, the accuracy of GROTOLAM translation is tested by comparing results of a fixed molecular dynamics configuration as obtained by both GROMACS (original case) or LAMMPS (GROTOLAM conversion).

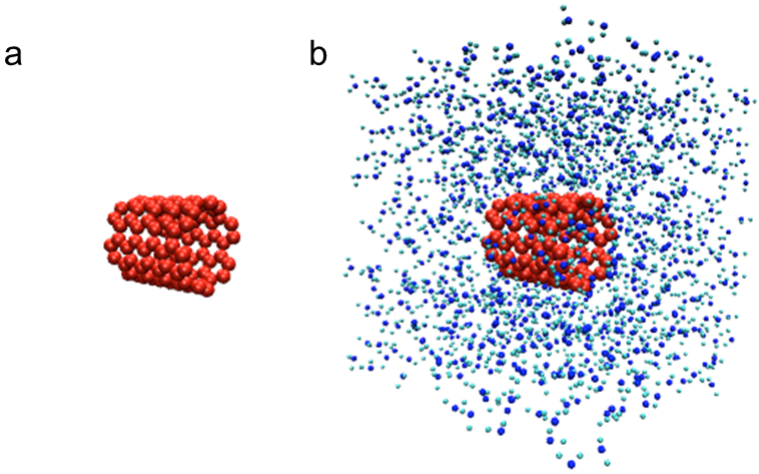

Figure D.2.: The CNT analyzed for the GROTOLAM benchmark. The CNT is shown (a) in void and (b) in a SPC/E water box.

The benchmark system consists in a short carbon nanotube ((5,5) CNT, 108 atoms) solvated by 930 molecules of SPC/E water. Here, the quantities to be compared for assessing the accuracy of GROTOLAM conversion are the different contributes to the total energy of the system during the molecular dynamics simulation. The considered Lennard-Jones parameters are $\sigma = 3.55\,\text{Å}$ and $\epsilon = 0.06983$ kcal mol^{-1} for carbon atoms [145], $\sigma_{OO} = 3.166\,\text{Å}$ and $\epsilon = 0.15535$ kcal mol^{-1} for water [156]. Partial charges of SPC/E water model are $q_O = -0.8476$ e and $q_H = 0.4238$ e, respectively [156]. Carbon-carbon bonds are modeled by harmonic potential, with equilibrium distance 1.42 Å and energy constant 572.0258 kcal Å^{-2} mol^{-1} [145]. CNT angle interactions are also described by harmonic potential, with equilibrium angle 120° and energy constant 67.1524 kcal rad^{-2} mol^{-1} [145]. For the sake of simplicity, dihedrals are not considered. Bond potentials of water molecules are represented following the standards of SPC/E model, namely bond equilibrium distance 1 Å and equilibrium angle 109.47°. Both bonds and angle of water molecules are constrained by SHAKE algorithm [351].

Van der Waals interactions are handled by 12-6 Lennard-Jones potential, while electrostatic interactions by Coulomb potential. PME and PPPM methods are used in GROMACS and LAMMPS for considering the long

range terms of the electrostatic interactions, respectively. The cut-off radius for the nonbonded interactions is set to 15 Å, while the skin distance for the neighbors to 2 Å and the neighbor list is updated every timestep. Boundary conditions are applied along all Cartesian directions. After the initialization of atom velocities by Maxwell-Boltzmann distribution (300 K), production runs are performed in NVT ensemble (Berendsen thermostat at 300 K; dumping factor at 100 fs; 1000000 steps; 0.1 fs timestep). Energies are stored every 100 steps and post-processed by MATLAB®.

Figure D.3 presents the measured trends of (a) bond, (b) angle, (c) Coulomb and (d) van der Waals interaction energies, both in case of GROMACS (red lines) and LAMMPS (blue lines) simulations. Altough an accurate agreement of energy values thus of GROTOLAM conversion performances is already noticeable from Figure D.3, a more quantitative comparison is made by evaluating the ratio between overall equilibrium energies in case of either LAMMPS or GROMACS simulations, namely

$$R_E = \frac{E_{LAMMPS}}{E_{GROMACS}}. \tag{D.1}$$

Quantity	R_E
Bond Potential Energy	1.0036
Angle Potential Energy	1.0067
Van Der Waals Energy	1.0047
Coulombic Energy	1.0032
Potential Energy	1.0025
Total Energy	1.0034

Table D.1.: Ratio between energies computed by either GROMACS (original case) or LAMMPS (GROTOLAM conversion), for the molecular dynamics setup in Figure D.2.

As shown in Table D.1, an accurate correspondence (i.e. less than 1% difference) between the outputs of the two simulators is found for all the physical quantities investigated. Hence, the benchmark validates the translation accuracy of GROTOLAM.

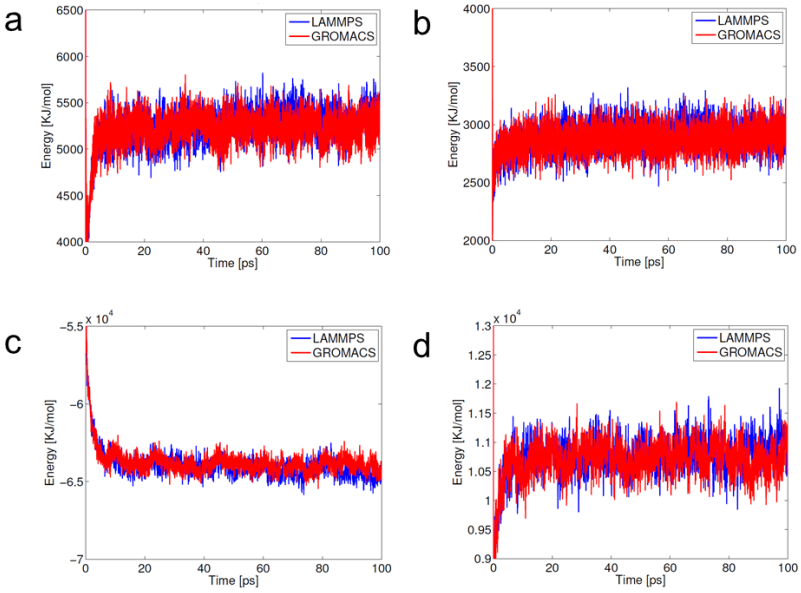

Figure D.3.: Comparison between energies computed by LAMMPS (blue lines) and GROMACS (red lines). (a) Bond, (b) angle, (c) Coulomb and (d) van der Waals interaction energies.

E. Details of Gd(DOTA) experiments

In this Appendix, further analyses of molecular dynamics and *in vitro* experiments of Gd(DOTA)-based contrast agents are detailed, starting from the data available in Reference [566]. First, tumbling times of the SiMP and SiP particles synthesized by Gizzatov and colleagues are estimated [566]. Second, power spectra of the simulated Gd(DOTA) molecules are reported, according to the Lipari-Szapo formalism. Finally, experimental data for Gd(DOTA)-SiMP contrast agents are analyzed, in order to compute the mean pore surface coverage of Gd(DOTA) molecules.

Tumbling time of SiP/SiMP particles

Molecular dynamics simulations of a Gd(DOTA) molecule chemically bonded to silica wall, which mimics the surface of a larger silicon nonporous (SiP) or mesoporous particle (SiMP), show that the bulk rotational correlation time of Gd(DOTA) in bulk water is not sufficient to fully describe the overall tumbling motion of complex MRI contrast agents such as those in Reference [566]. Hence, in this Section τ_R of micrometer spherical and disk-like particles is estimated by means of Stoke-Einstein relation.

According to Stokes-Einstein's relation for Brownian motion, the rotational diffusion coefficient (D_R) and the molecular correlation time (τ_M) for an isotropic particle are correlated by the classical formula:

$$\tau_M = \frac{1}{6D_R}, \tag{E.1}$$

where D_R is inversely proportional to the rotational drag coefficient (γ_R), namely

$$D_R = \frac{k_B T}{\gamma_R}, \tag{E.2}$$

being k_B the Boltzmann constant and T the environment temperature.

In case of spherical particles [14]

$$\gamma_R = 8\mu\pi r_p^3, \tag{E.3}$$

where μ is the dynamic viscosity of the surrounding media and r_p is the particle radius.

When cylindrical geometries (diameter Φ, length L; axial ratio $p = L/\Phi$) are considered instead, the tumbling ($\tau_M^{\perp}$) and spinning ($\tau_M^{\parallel}$) molecular correlation times are related to the rotational motion transversal or longitudinal to the cylinder length, respectively:

$$\tau_M^{\perp} = \frac{1}{4D_R^{\perp}} \tag{E.4}$$

$$\tau_M^{\parallel} = \frac{1}{2D_R^{\parallel}}. \tag{E.5}$$

In case of disk-like particles, rotational diffusion coefficients can be evaluated as [601]:

$$D_R^{\perp} = \frac{1}{6\tau_a} \tag{E.6}$$

$$D_R^{\parallel} = \frac{1}{\tau_b} - \frac{5}{6\tau_a}, \tag{E.7}$$

where for $p < 0.75$

$$\begin{aligned} \tau_a &= \tau_0(1.18 + 0.1744(\ln p + 0.2877)^2 - 0.2417(\ln p + 0.2877)^3 + \\ &\quad -3.882 \times 10^{-2}(\ln p + 0.2877)^4) \end{aligned} \tag{E.8}$$

$$\begin{aligned} \tau_b &= \tau_0(1.183 + 0.2902\,(\ln p) + 0.4406(\ln p)^2 - 5.850 \times 10^{-2}(\ln p)^3 + \\ &\quad -9.544 \times 10^{-3}(\ln p)^4), \end{aligned} \tag{E.9}$$

and $\tau_0 = \frac{\pi L^3 \mu}{4p^2 k_B T}$ is the rotational time for a sphere with the same volume of the disk.

In the experimental results shown by Gizzatov and colleagues [566], spherical nonporous Silica Particles (SiP) with diameter $\Phi_{SiP} = 1000$ nm and discoidal Silicon Mesoporous Particles (SiMP) with diameter $\Phi_{SiMP} = 1000$ nm and length $L = 400$ nm are analyzed. If bulk conditions are considered for the solvent (i.e. dynamic viscosity $\mu \cong 1 \times 10^{-3}$ Pa s at 310 K, Equation E.1 implies $\tau_{M,SiP} = 0.13$ s, whereas Equation E.4 and E.5 $\tau_{M,SiMP}^{\perp} = 0.15$ s and $\tau_{M,SiMP}^{\parallel} = 0.32$ s, respectively.

Power spectra of simulated Gd(DOTA)

Once the characteristic τ_E of Gd(DOTA) bonded to a silica wall and τ_M of SiMP are estimated, it can be demonstrated that the spectral density of the overall contrast agent can be determined from Equation 6.6 as

$$J(\omega) = \frac{S^2 \tau_M}{1 + \omega^2 \tau_M^2} + \frac{\left(1 - S^2\right) \tau_T}{1 + \omega^2 \tau_T^2}, \tag{E.10}$$

where ω represents a frequency and $\tau_T^{-1} = \tau_M^{-1} + \tau_E^{-1}$. The spectral density of a complex is related to its NMR relaxation response, because it influences the relaxation time of water protons in the first coordination sphere. The formalism proposed by Lipari and Szabo has proved to be accurate for the analysis of NMR relaxation data, and it is a *de facto* standard method because of its simplicity [602].

First, Equation E.10 is applied to the case of a Gd-based complex characterized by isotropic tumbling motion (i.e. $S^2 = 0$, $\tau_T = \tau_R = \tau_{R,bulk}$) but different $\tau_{R,bulk}$ (i.e. 10 ps, 75 ps, 1 ns, 100 ns and 1000 ns), in order to assess the effect of tumbling time of contrast agents on $J(\omega)$, thus on their NMR relaxation response. Results in Figure E.1 show that the spectral density monotonically increases with τ_R for $\omega < 10$ MHz, whereas the latter relation progressively inverts at larger frequencies (i.e. $\omega > 10000$ MHz). Hence, in clinically relevant frequencies (i.e. 0.25–3 T, namely 10–130 MHz) the relation $J(\omega) \sim \tau_R$ holds only for $\tau_R < 1$ ns (Figure E.2), whereas further increments of τ_R have detrimental effects on $J(\omega)$.

Second, Equation E.10 is applied to the case of Gd(DOTA) bonded to SiMP at different distances d_{min} from the pore surface, namely 0.23, 0.26 and 2 nm respectively. S^2 and τ_E of Gd(DOTA) are taken from MD results in Table B.12, whereas $\tau_{M,SiMP}^{\perp} = 0.15$ s as from Equation E.4. Results in Figure E.3 show that Gd(DOTA) and Gd(DOTA)+SiMP at $d_{min} = 2$ nm have the same spectral density, i.e. the effect of SiMP bonding is not noticeable on $J(\omega)$ if the wall-DOTA bond is large thus $S^2 \to 0$. Moreover, for clinically relevant frequencies, the bonding of Gd(DOTA) to larger particles have different impacts on $J(\omega)$ according to the distance between Gd(DOTA) and the particle surface (Figure E.4): $J(\omega)$ increases respect the case of bulk Gd(DOTA) for $d_{min} > 0.26$ nm, whereas it decreases for $d_{min} < 0.26$ nm (molecule blocked on the surface).

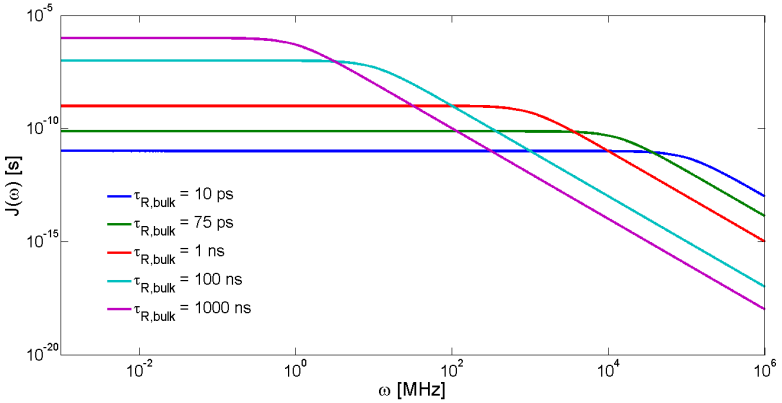

Figure E.1.: Spectral densities of Gd-based contrast agents immersed in bulk water with increasing tumbling times ($\tau_{R,bulk}$).

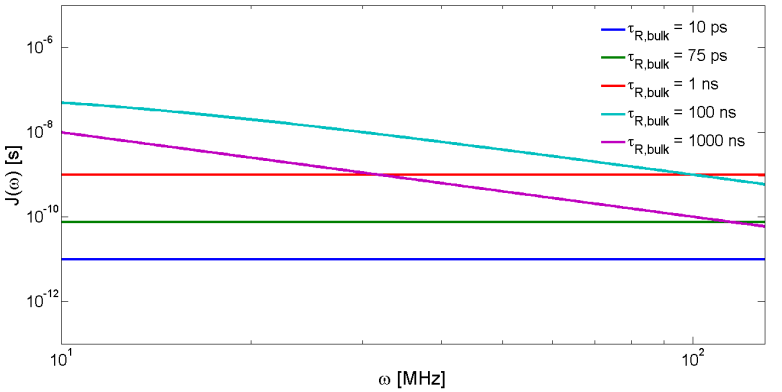

Figure E.2.: Spectral densities of Gd-based contrast agents immersed in bulk water with increasing tumbling times $\tau_{R,bulk}$, focusing on clinically-relevant conditions (i.e. 10–130 MHz).

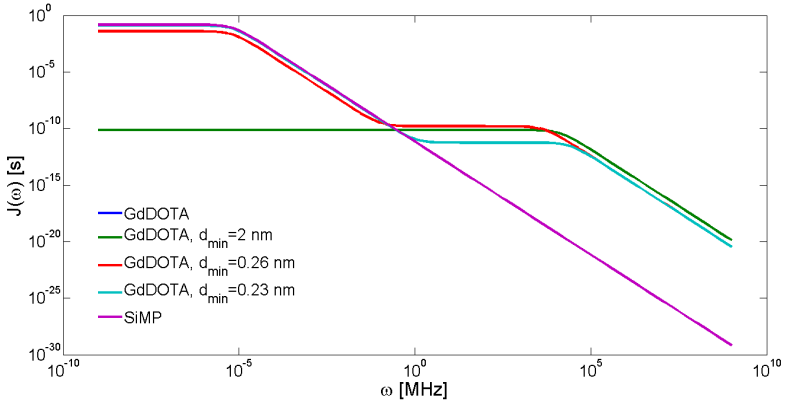

Figure E.3.: Spectral densities of Gd(DOTA) bonded to SiMP at different distances from the pore surface. Spectral densities of SiMP and Gd(DOTA) alone are also shown. Note that $J(\omega)$ of Gd(DOTA) and Gd(DOTA)+SiMP at $d_{min} = 2$ nm are overlapped.

Experimental pore surface coverage by Gd(DOTA)

For a better understanding of the difference between the measured relaxivities of Gd(DOTA)+SiMP-HP and SP [566], the surface density of Gd(DOTA) molecules on the SiMP-HP and SP surfaces is calculated from the experimental data kindly provided by Gizzatov and colleagues. First, the surface (S_p) and volume (V_p) of a SiMP nanopore (Φ_{SiMP} particle diameter, L height, ϕ pore diameter) are calculated as

$$S_p = \pi \frac{\phi}{2} L \tag{E.11}$$

and

$$V_p = \pi \frac{\phi^2}{4} L, \tag{E.12}$$

respectively. Then, the external surface of SiMP ($S_{e,SiMP}$) is obtained as

$$S_{e,SiMP} = 2\left(\pi \frac{{\Phi_{SiMP}}^2}{4}\right) + \pi \Phi_{SiMP} L - 2N_p \left(\pi \frac{\phi^2}{2}\right), \tag{E.13}$$

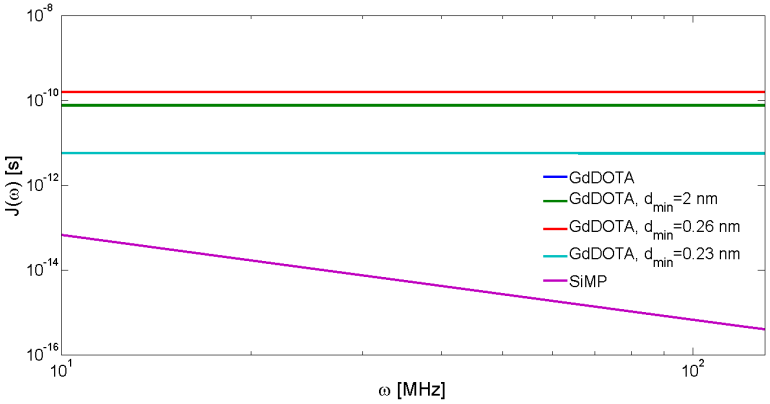

Figure E.4.: Spectral density of Gd(DOTA) bonded to SiMP at different distances from the pore surface, focusing on clinically-relevant conditions (i.e. 10–130 Hz). Spectral densities of SiMP and Gd(DOTA) alone are also shown. Note that $J(\omega)$ of Gd(DOTA) and Gd(DOTA)+SiMP at $d_{min} = 2$ nm are overlapped.

where $N_p = \frac{\varrho_p V_{SiMP}}{V_p}$ is the number of SiMP's nanopores, $V_{SiMP} = \pi \frac{\Phi_{SiMP}{}^2}{4} L$ the volume of the SiMP and ϱ_p its porosity. Hence, the overall accessible surface of the mesoporous silicon particle is

$$S_{t,SiMP} = N_p S_p + S_{e,SiMP}. \tag{E.14}$$

The surface density of Gd(DOTA) on the accessible surface of the SiMP is then estimated as

$$\rho_{Gd(DOTA)} = \frac{[Gd]\, V_{sol} N_A}{N_{SiMP} S_{t,SiMP}}, \tag{E.15}$$

where $[Gd]$ is the molar concentration of Gd(DOTA) bonded to SiMPs in an experimental sample, V_{sol} is the sample volume, N_{SiMP} the amount of SiMP particles in the sample and N_A the Avogadro number. Hence, the percentage of $S_{t,SiMP}$ covered by Gd(DOTA) molecules is

$$\gamma_{Gd(DOTA)} = \left(\rho_{Gd(DOTA)} S_{Gd(DOTA)}\right) \cdot 100, \tag{E.16}$$

with $S_{Gd(DOTA)}$ the equivalent Gd(DOTA) occupancy area; whereas the

average barycenter distance between contiguous Gd(DOTA) can be estimated as

$$\overline{l_{Gd-Gd}} = \left(\rho_{Gd(DOTA)}\right)^{-\frac{1}{2}}. \tag{E.17}$$

Table E.1 reports the initial data for Equations E.11 to E.17, whereas Tables E.2 and E.3 the results obtained in case of SiMP-HP and SP. Based on the variance of experimental measurements, two extreme approximations are considered as N_{SiMP} within the analyzed sample, namely 1×10^8 and 5×10^8.

	HP	**SP**
Φ_{SiMP} [nm]	1000	1000
ϕ [nm]	50	10
L [nm]	400	400
ϱ_p [-]	0.6	0.6
S_p [nm^2]	6.54E+04	1.26E+04
V_p [nm^3]	1.13E+06	3.14E+04
$[Gd]$[mM]	0.00186	0.00217
V_{sol}[mL]	5	5
$S_{Gd(DOTA)}$[nm^2]	0.79	0.79

Table E.1.: Geometry of SiMP-HP and SP nanoparticles and concentration of Gd(DOTA) therein.

	HP	**SP**
$\rho_{Gd(DOTA)}[\#/n\text{m}^2]$	3.88	0.85
$\gamma_{Gd(DOTA)}$ [%]	304	66
$\overline{l_{Gd-Gd}}$ [nm]	0.51	1.09

Table E.2.: Gd(DOTA) surface distribution and coverage if $N_{SiMP} =$ 1.0E8 is considered.

	HP	**SP**
$\rho_{Gd(DOTA)}[\#/n\text{m}^2]$	0.78	0.17
$\gamma_{Gd(DOTA)}$ [%]	61	13
$\overline{l_{Gd-Gd}}$ [nm]	1.14	2.43

Table E.3.: Gd(DOTA) surface distribution and coverage if $N_{SiMP} =$ 5.0E8 is considered.