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Surface properties of calcinated titanium dioxide probed by solvatochromic indicators:

Relevance to catalytic applications

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Figure SI-1: Snapshot of one of the conformations calculated by MC simulation, showing BuPMBBr₂ surround by the first solvation shell of methanol molecules.

Figure SI-2: Snapshot of one of the conformations calculated by MC simulation, showing BuPMBBr₂ surround by the first solvation shell of diethyl ether molecules.

Figure SI-3: Molecular structure and atom numbering of BuPMBBr₂.

Table SI-1 – X,Y and Z coordinates, charge (q) and Lennard-Jones ϵ and σ parameters of BuPMBBr₂ atoms employed in the *ab-initio* and Monte Carlo simulations.

Atom label	X, Å	Y, Å	Z, Å	q, e ⁻	ϵ , kcal mol ⁻¹	σ , Å
O1	-5.234159	0.195988	0.305685	-0.615273	0.17	3.07
C2	-4.026474	0.066005	0.161088	1.074551	0.07	3.55
C3	-3.089113	1.205468	0.056927	-0.603354	0.07	3.55
C4	-1.749954	1.069156	-0.104747	0.268808	0.07	3.55
C5	-1.139491	-0.227737	-0.185539	-0.079144	0.07	3.55
C6	-2.003956	-1.369204	-0.088624	0.043079	0.07	3.55
C7	-3.344682	-1.237595	0.071642	-0.472295	0.07	3.55
C8	0.232487	-0.426520	-0.350863	-0.063563	0.076	3.55
C9	1.237761	0.539486	-0.471184	-0.534653	0.076	3.55
C10	2.599787	0.279477	-0.636632	0.491693	0.11	3.75
C11	3.545166	1.357604	-0.756942	-0.377701	0.11	3.75
C12	4.875196	1.134276	-0.920322	-0.090090	0.11	3.75
N13	5.397022	-0.134681	-0.982184	0.216558	0.17	3.25
C14	4.531799	-1.195960	-0.876913	-0.152472	0.11	3.75

C15	3.193796	-1.031487	-0.713081	-0.299243	0.11	3.75
C16	6.844068	-0.368025	-1.120433	-0.328507	0.066	3.5
C17	7.543889	-0.750513	0.189322	0.153997	0.066	3.5
C18	7.530089	0.340429	1.265572	0.154941	0.066	3.5
C19	8.276328	-0.074981	2.536695	-0.398845	0.066	3.5
Br20	-3.866768	2.946533	0.163413	-0.023870	0.47	3.47
Br21	-4.453597	-2.787723	0.192843	-0.047120	0.47	3.47
H4	-1.563112	-2.358071	-0.147331	0.098266	0.03	2.42
H6	-1.133764	1.956201	-0.172345	0.042630	0.03	2.42
H8	0.536930	-1.469538	-0.388559	0.137742	0.03	2.42
H9	0.955883	1.586523	-0.438927	0.216195	0.03	2.42
H11	2.583321	-1.921429	-0.648881	0.168498	0.03	2.42
H12	4.984302	-2.177063	-0.940912	0.177971	0.03	2.42
H14	5.588743	1.941687	-1.014631	0.146387	0.03	2.42
H15	3.194522	2.381621	-0.722305	0.187071	0.03	2.42
H16	7.279204	0.544770	-1.533361	0.123762	0.03	2.5
H16	6.983169	-1.155052	-1.866500	0.117816	0.03	2.5
H17	7.093342	-1.667987	0.586045	-0.016537	0.03	2.5
H17	8.580232	-1.005370	-0.062738	0.004960	0.03	2.5
H18	7.982755	1.253501	0.859060	-0.015843	0.03	2.5
H18	6.495643	0.594672	1.519961	-0.006788	0.03	2.5
H19	8.251986	0.720396	3.285388	0.112699	0.03	2.5
H19	7.827786	-0.966259	2.985695	0.096167	0.03	2.5
H19	9.325762	-0.301387	2.325393	0.091509	0.03	2.5