Supporting Information

Modelling the surface of amorphous dehydroxylated silica: the influence of the potential on the nature and density of defects.

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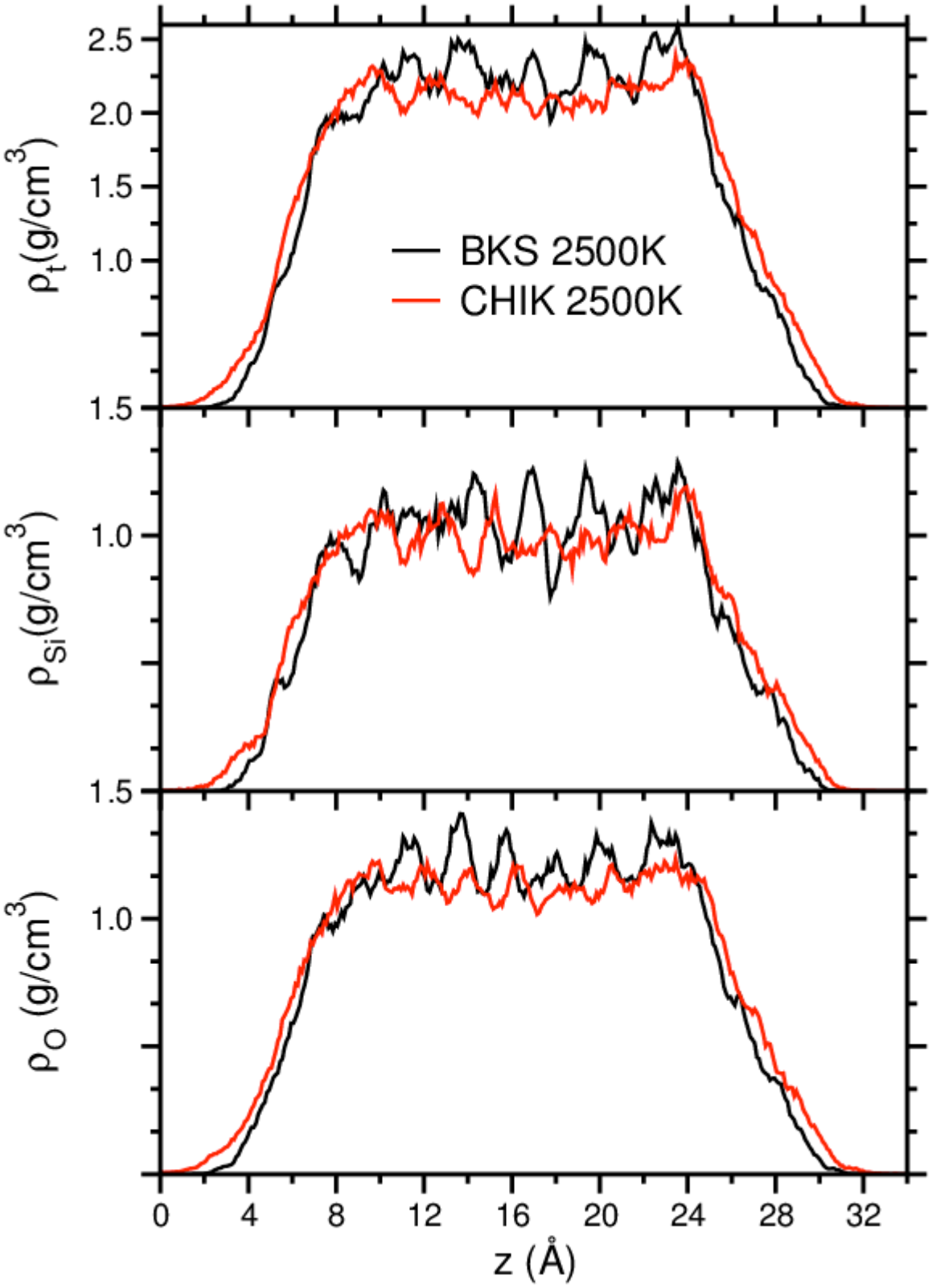

Figure S1: Density profiles ρ_t (t = Si and O), ρ_{Si} and ρ_O (black: BKS, red: CHIK) for the liquid film at 2500 K.

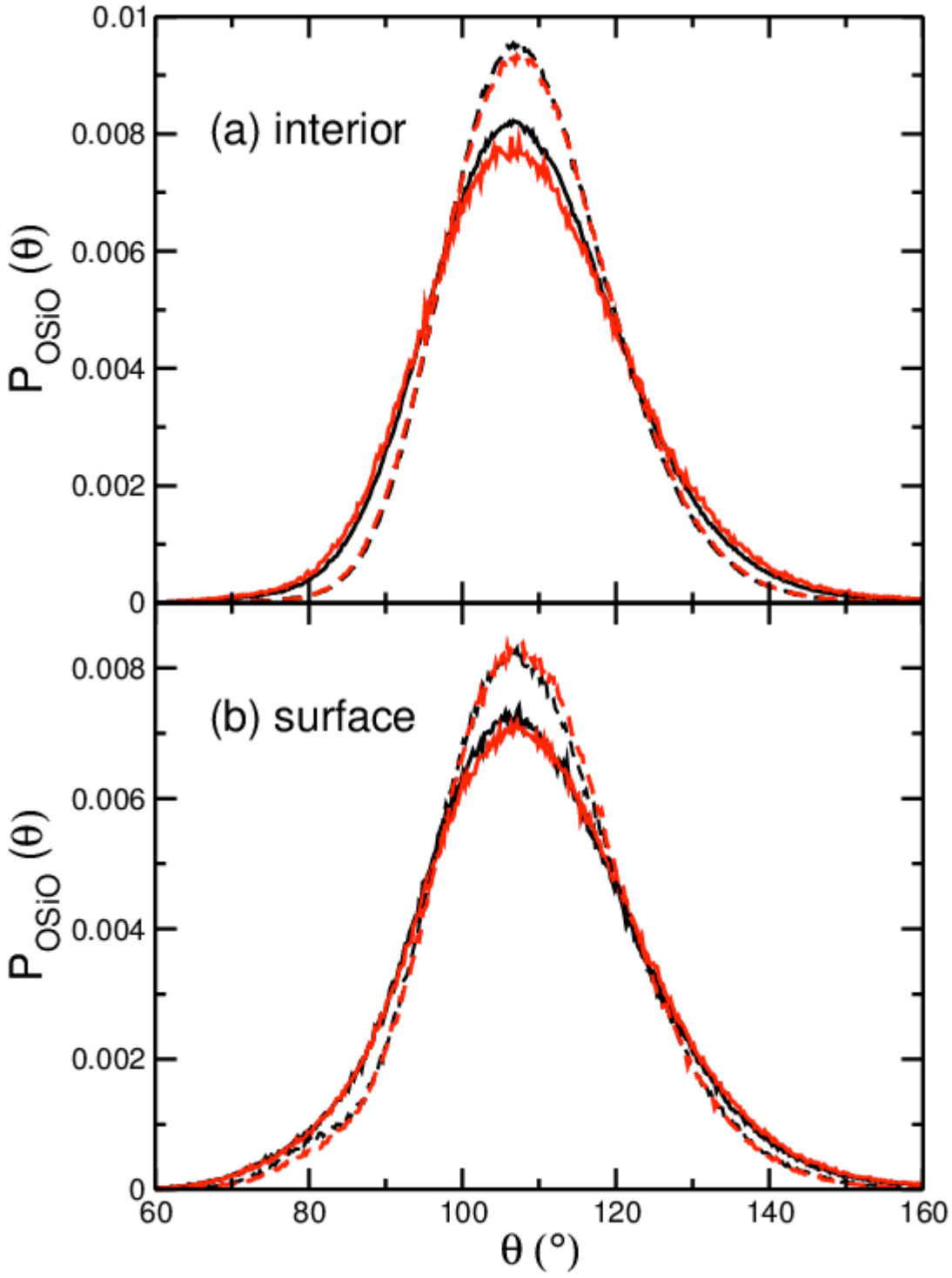

Figure S2: Angle distribution functions P_{osio} (black: BKS, red: CHIK) for the liquid film. The solid and dashed lines are for 3400 and 2500 K, respectively.

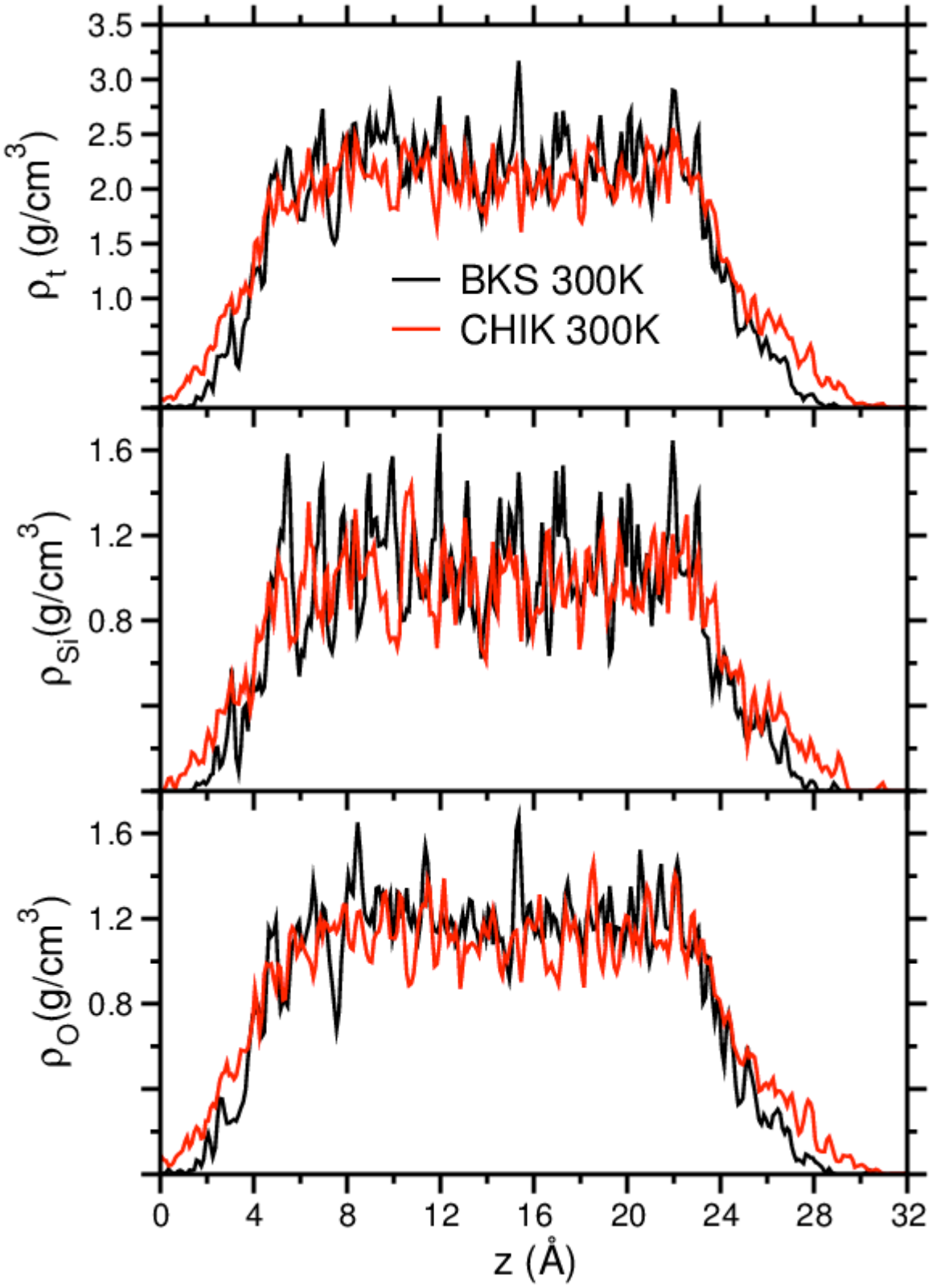

Figure S3: Density profiles ρ_t (t = Si and O), ρ_{Si} and ρ_O (black: BKS, red: CHIK) for the glass film at 300 K.

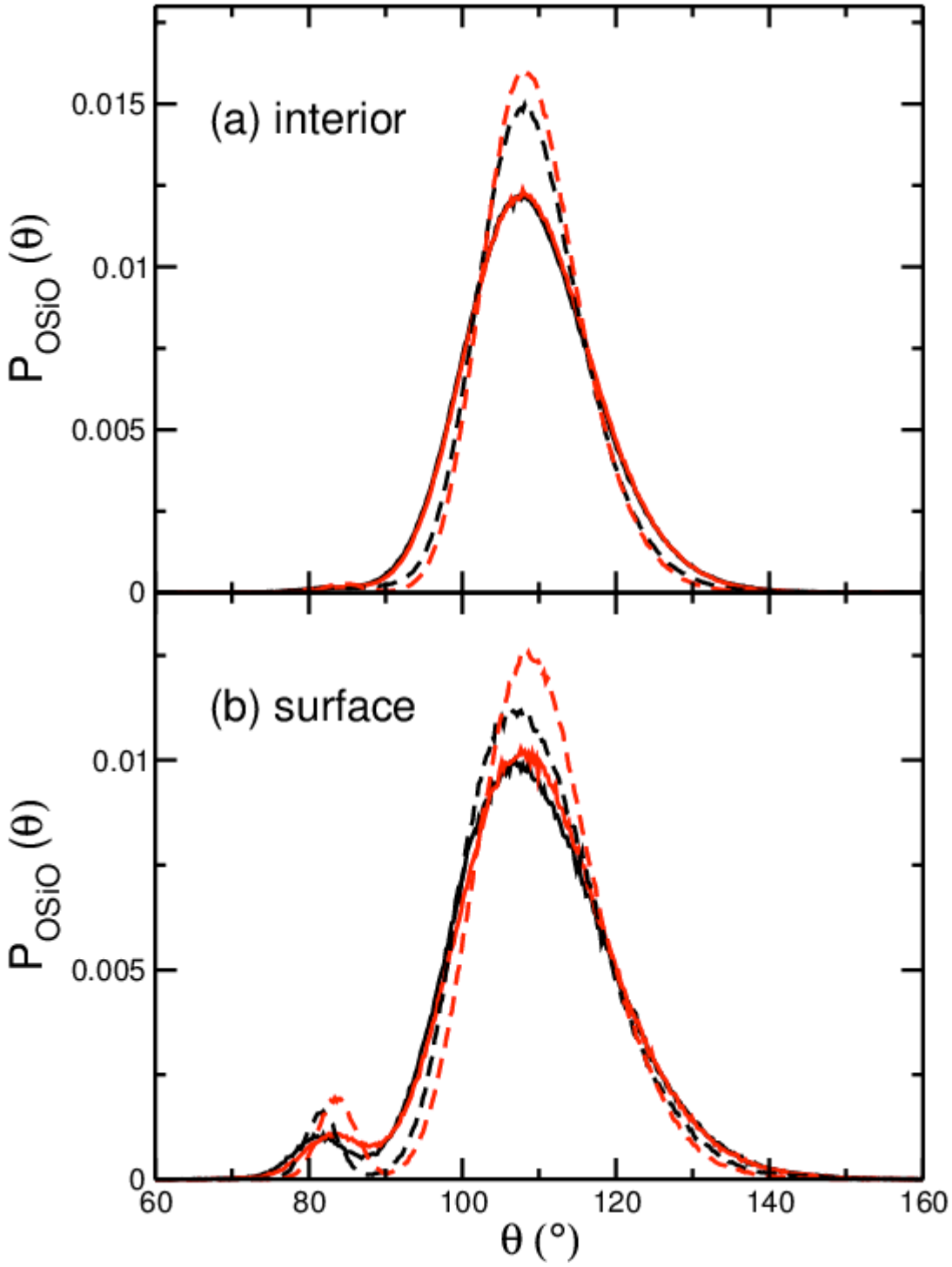

Figure S4: Angle distribution functions P_{osio} (black: BKS, red: CHIK) for the glass film. The solid and dashed lines are for 1000 and 300 K, respectively.

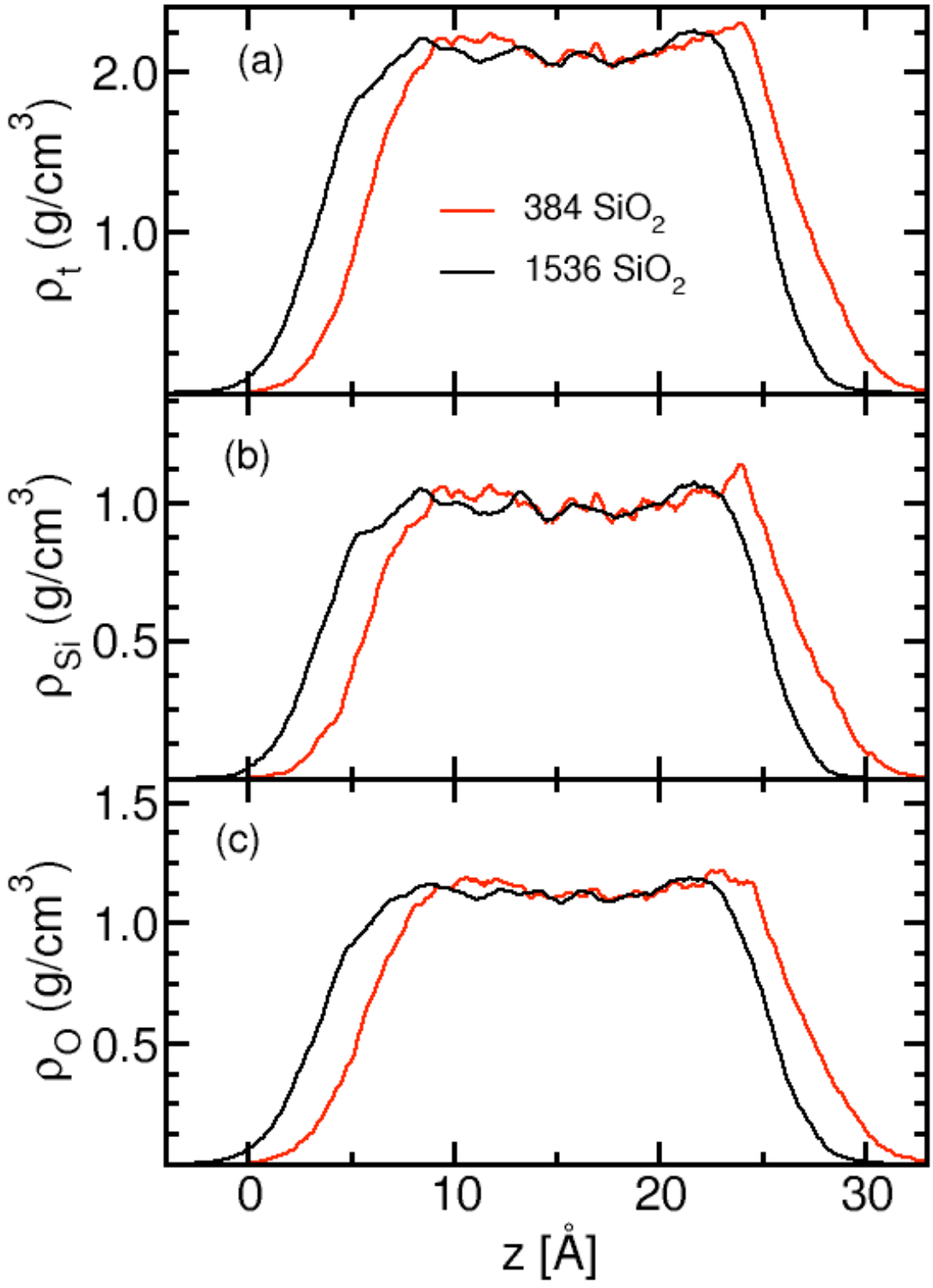

Figure S5: Density profiles ρ_t (t = Si and O), ρ_{Si} and ρ_O (black: large, red: small models) for the liquid film at 3400 K with CHIK.

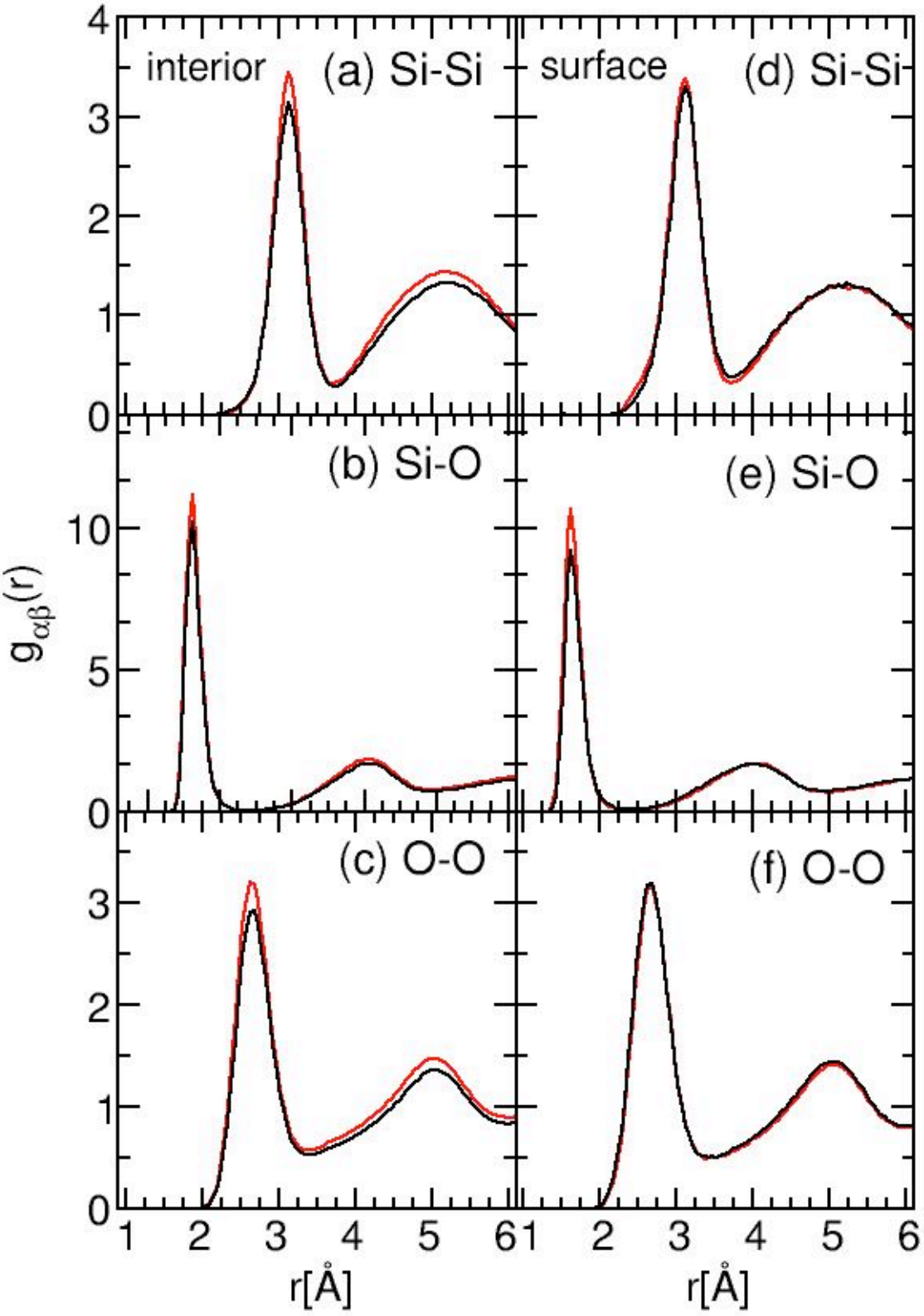

Figure S6: Radial distribution functions $g_{ij}(r)$ PDF (black: large, red: small models) for the liquid film at 3400 K with CHIK.

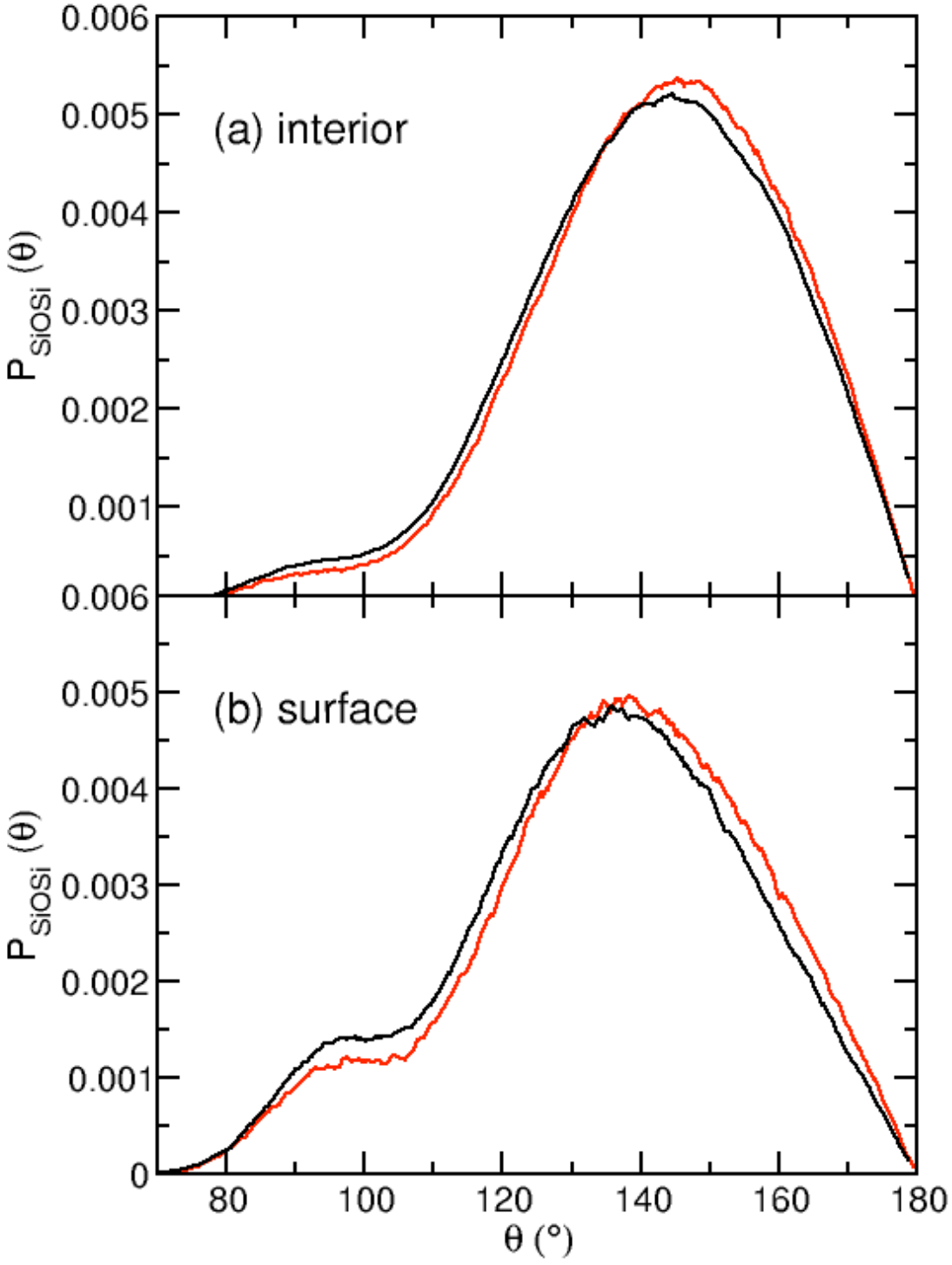

Figure S7: Angle distribution functions P_{SiOSi} (black: large, red: small models) for the liquid film at 3400 K with CHIK.

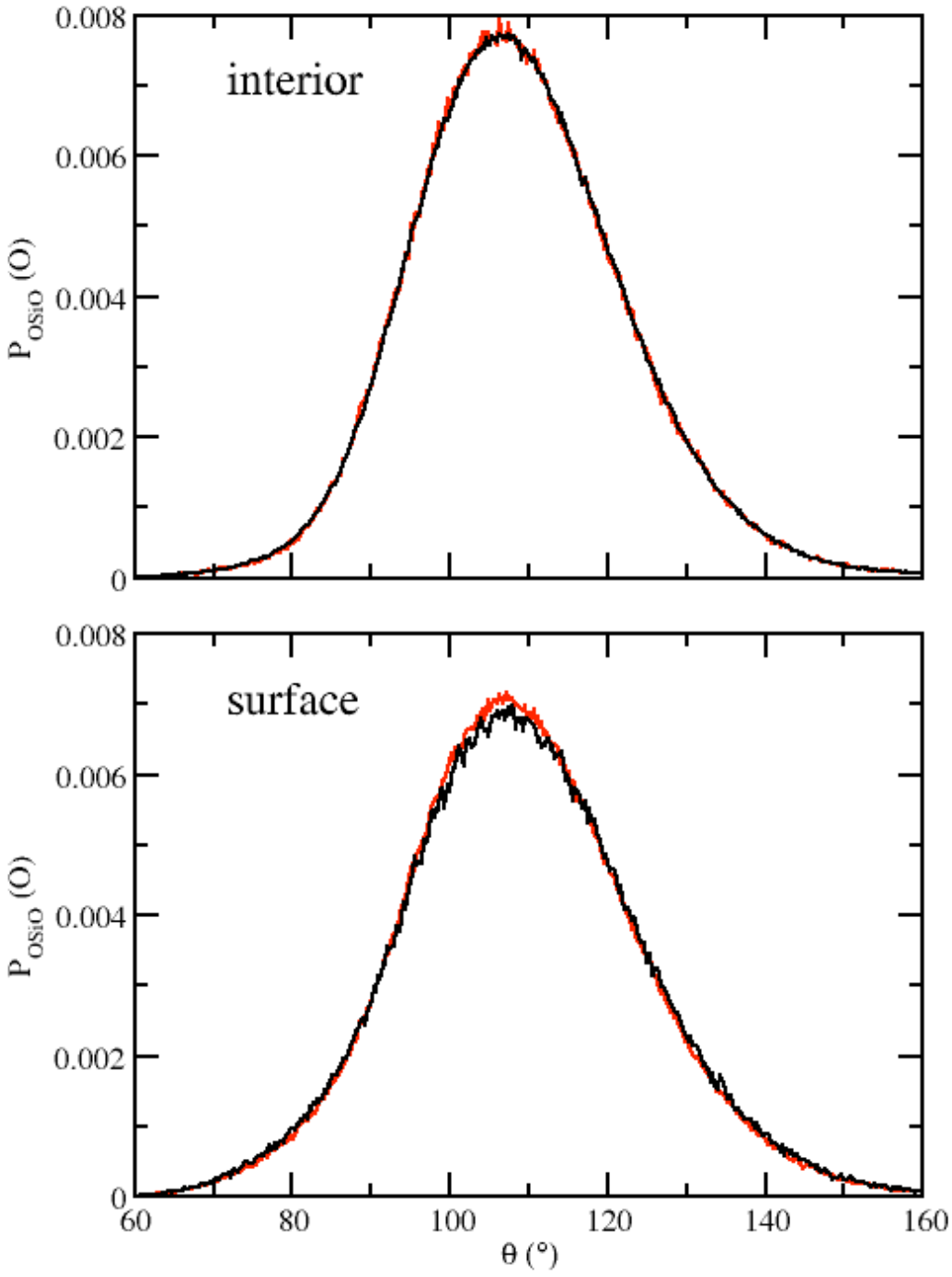

Figure S8: Angle distribution functions P_{osio} (black: large, red: small models) for the liquid film at 3400 K with CHIK.

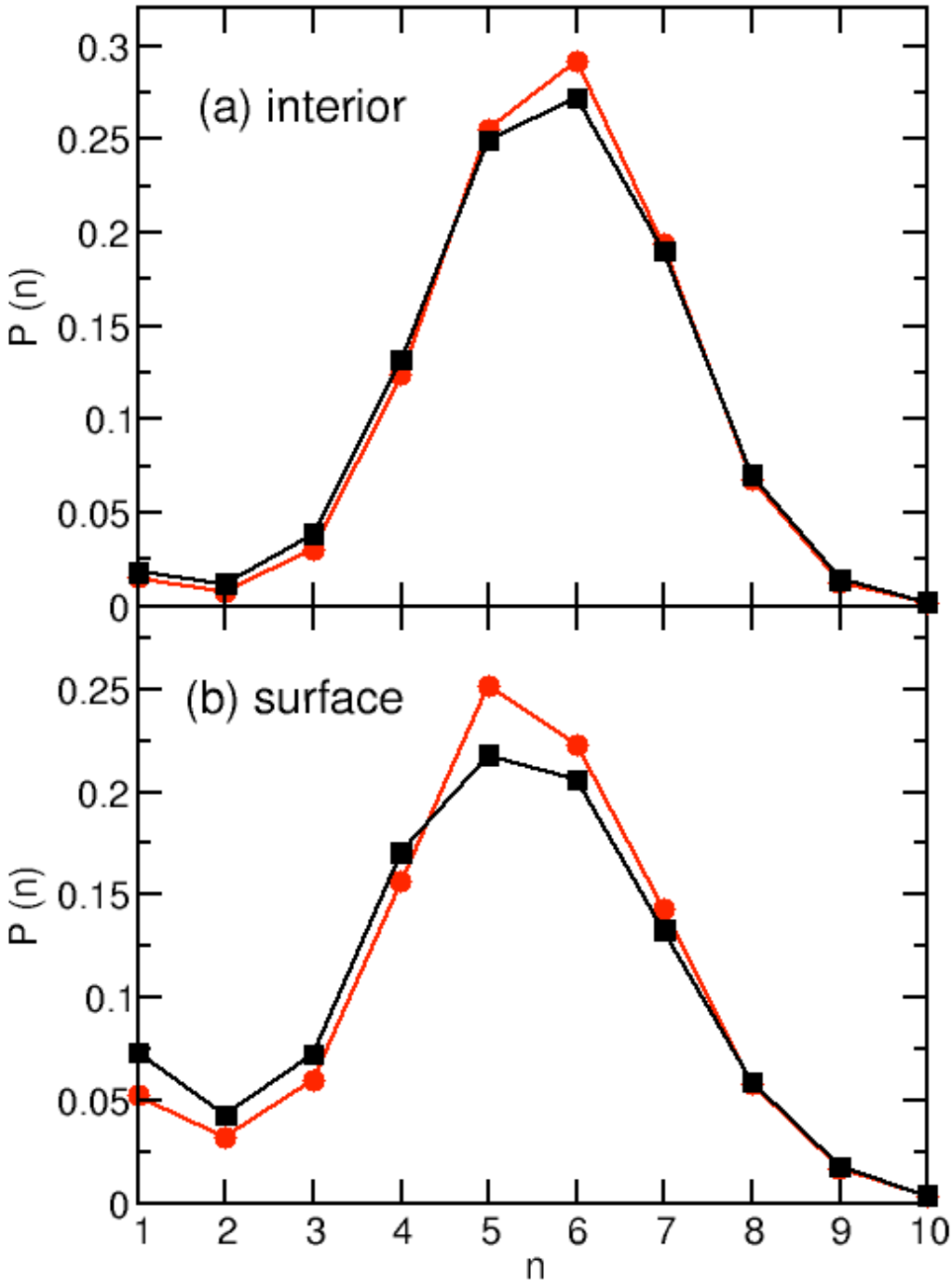

Figure S9: Distributions P(n) (black: large, red: small models) of $(SiO)_n$ type rings, nM, for the surface and interior of the liquid film at 3400 K with CHIK.

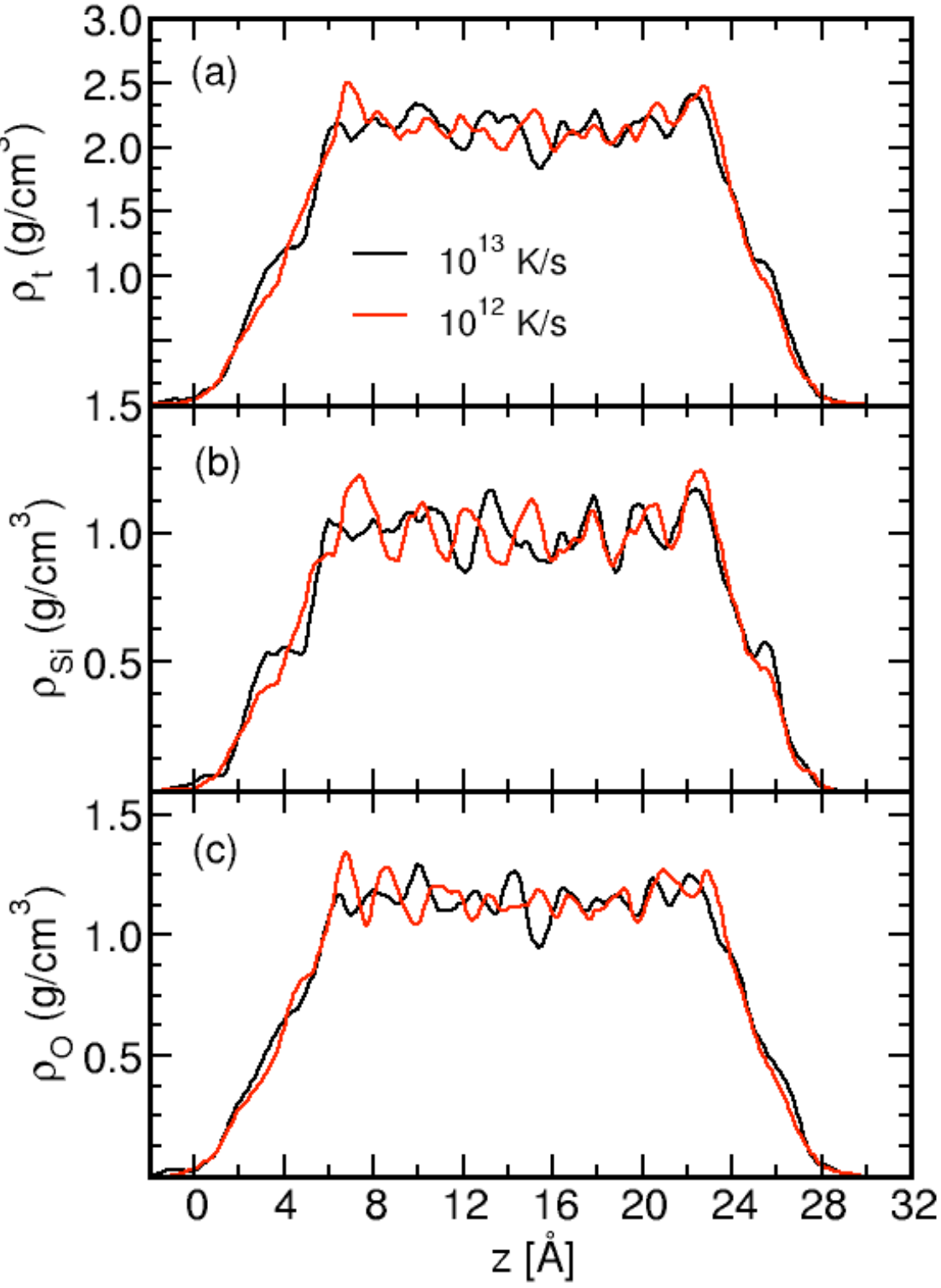

Figure S10: Density profiles ρ_t (t = Si and O), ρ_{si} and ρ_o (black: quenching rate of 10^{13} K/s, red: 10^{12} K/s) for the glass film at 1000 K with CHIK.

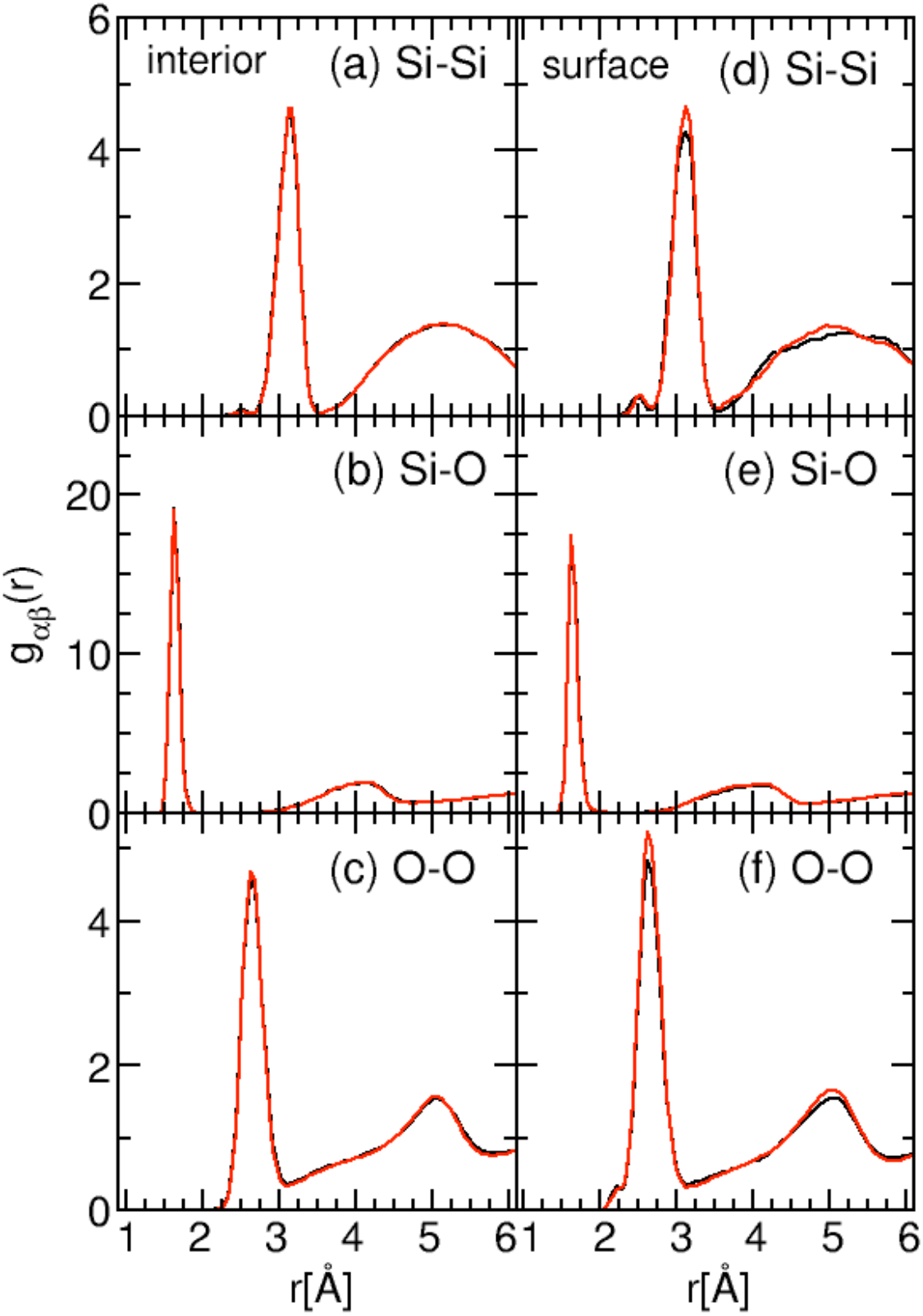

Figure S11: Radial distribution functions $g_{ij}(r)$ PDF (black: quenching rate of 10^{13} K/s, red: 10^{12} K/s) for the glass film at 1000 K with CHIK.

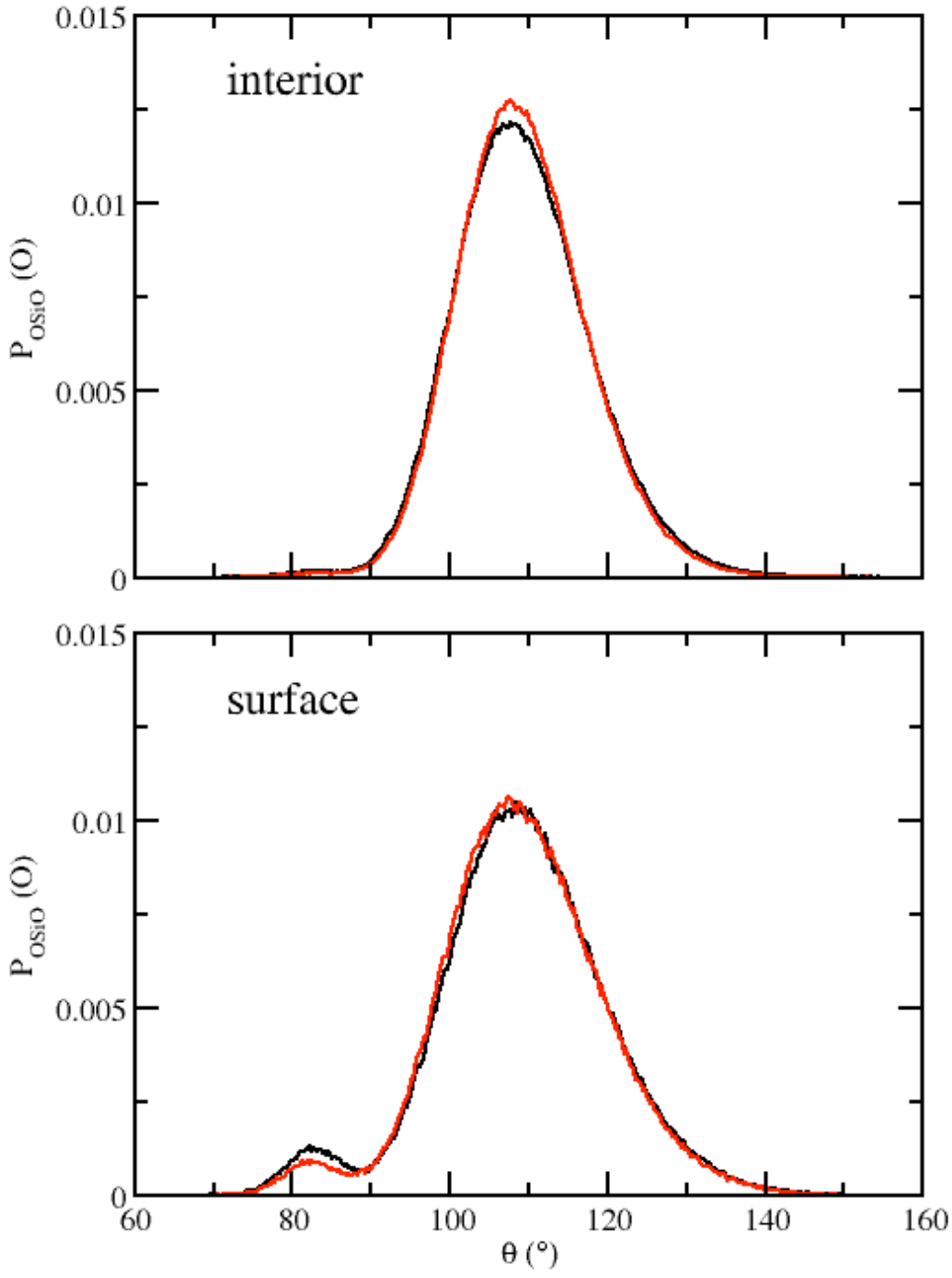

Figure S12: Angle distribution functions P_{osio} (black: quenching rate of 10^{13} K/s, red: 10^{12} K/s) for the glass film at 1000 K with CHIK.

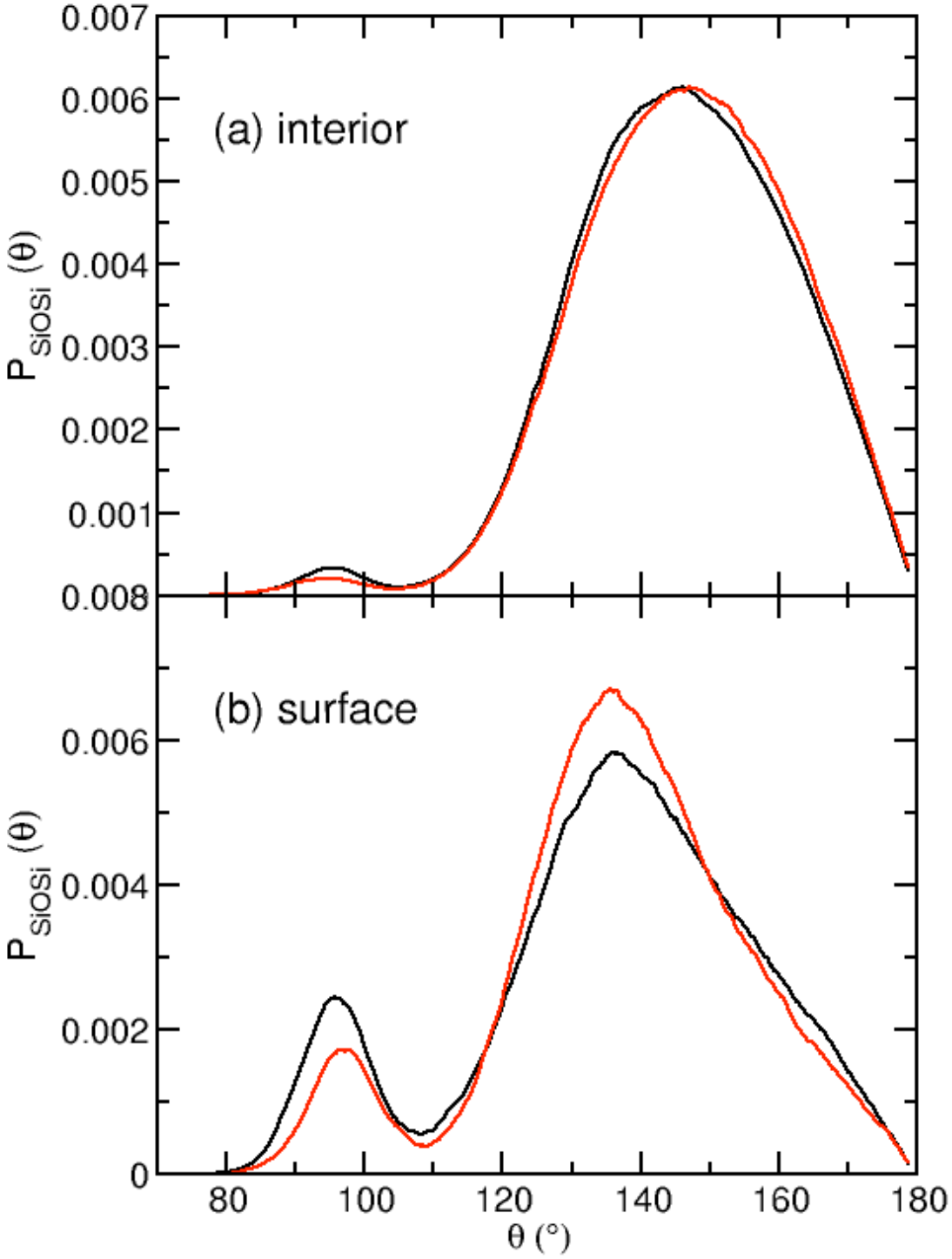

Figure S13: Angle distribution functions P_{siosi} (black: quenching rate of 10^{13} K/s, red: 10^{12} K/s) for the glass film at 1000 K with CHIK.

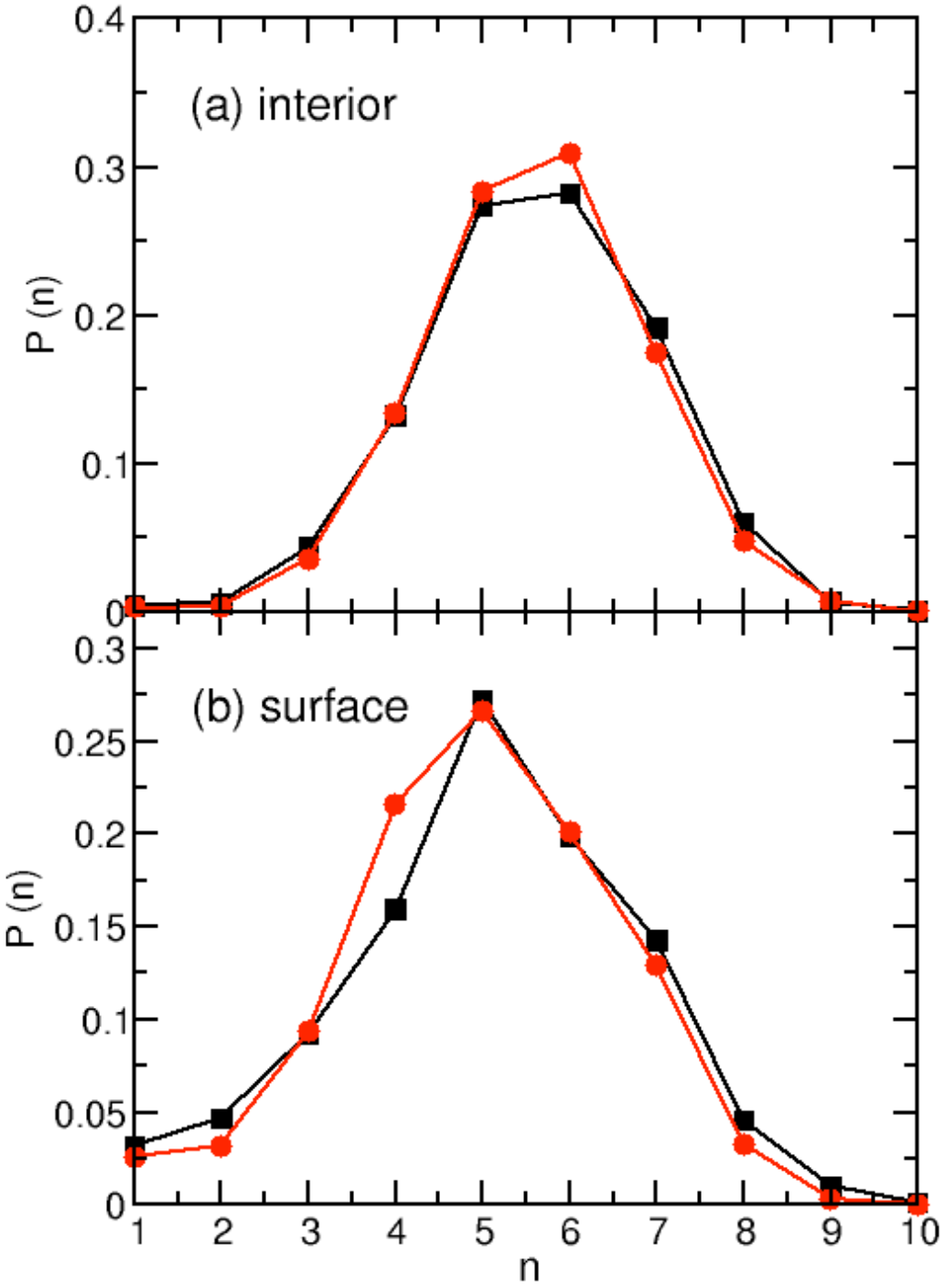

Figure S14: Distributions P(n) (black: quenching rate of 10^{13} K/s, red: 10^{12} K/s) of $(SiO)_n$ type rings, nM, for the surface and interior of the glass film at 1000 K with CHIK.

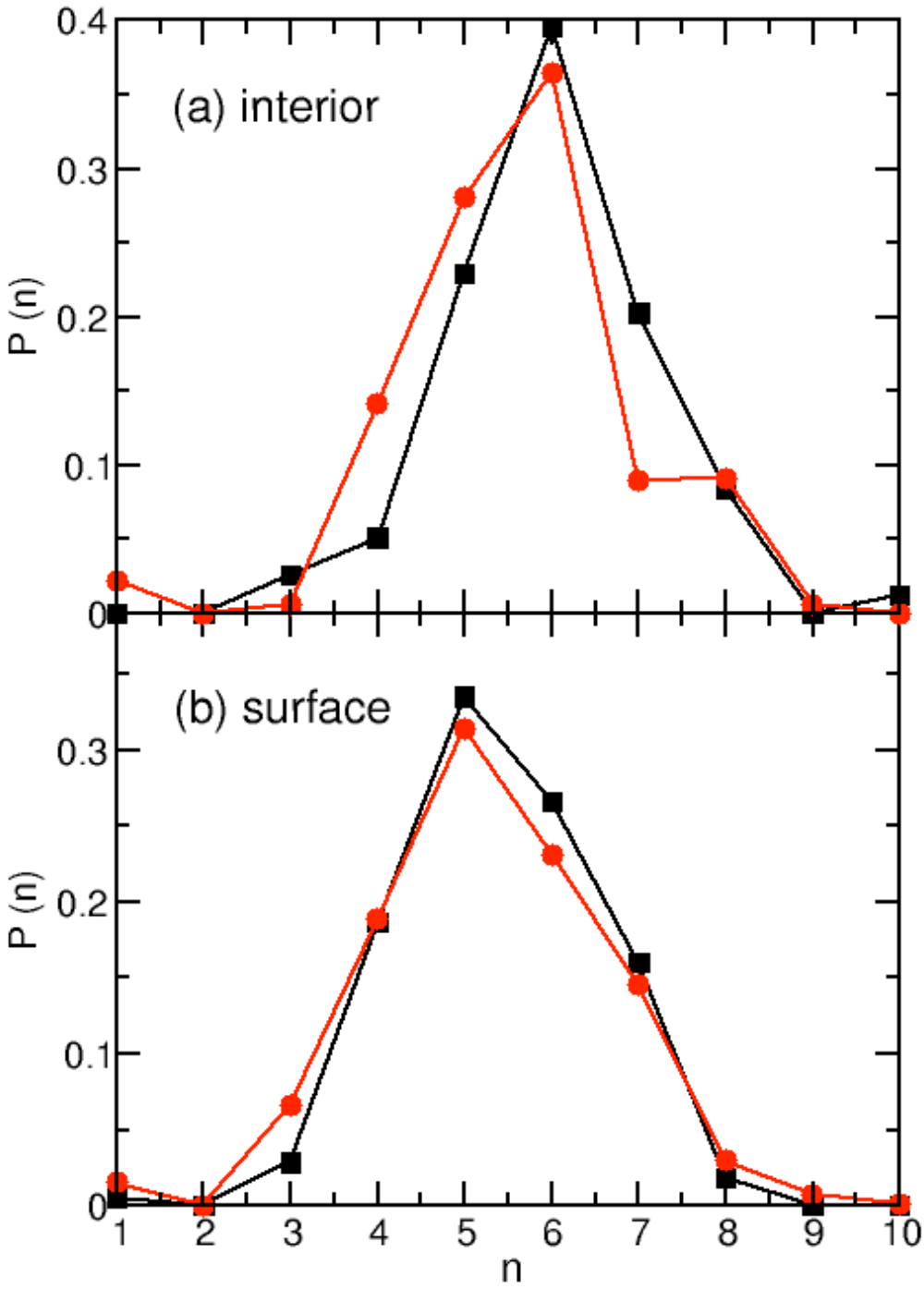

Figure S15: Distributions of $(SiO)_n$ ring lengths, nM, around the 2M rings for the interior and the surface of the glass film (black: BKS, red: CHIK) at 300 K.

Domain	BKS	CHIK

	T(K)	1000	300	1000	300
Interior	CN_{Si} (3)	0.1	0	2	0.9
	CN_{Si} (4)	97.8	98.2	97.9	99.1
	CN_{Si} (5)	2.1	1.8	0	0
	CN_{O} (1)	0.9	1.5	2.5	2.1
	CN_{O} (2)	98.9	98.5	97	97.4
	CN_{O} (3)	0.2	0	0.4	0.5
Surface	CN_{Si} (3)	1.2	1.0	2.9	3.5
	CN_{Si} (4)	98.2	98.5	97	96.5
	CN_{Si} (5)	0.6	0.5	0.1	0
	CN_{O} (1)	2	1.9	5.7	6.4
	CN_{O} (2)	96.6	96.5	91.7	90.9
	CN_{O} (3)	1.4	1.6	2.7	2.7

Table S16: Percentages of the Si and O Coordination Numbers (CN) located in a sphere of radius 4 Å from 2M rings.