Study on the adsorption mechanisms of NH3, H2S, and SO2 on sepiolite via molecular dynamics simulations

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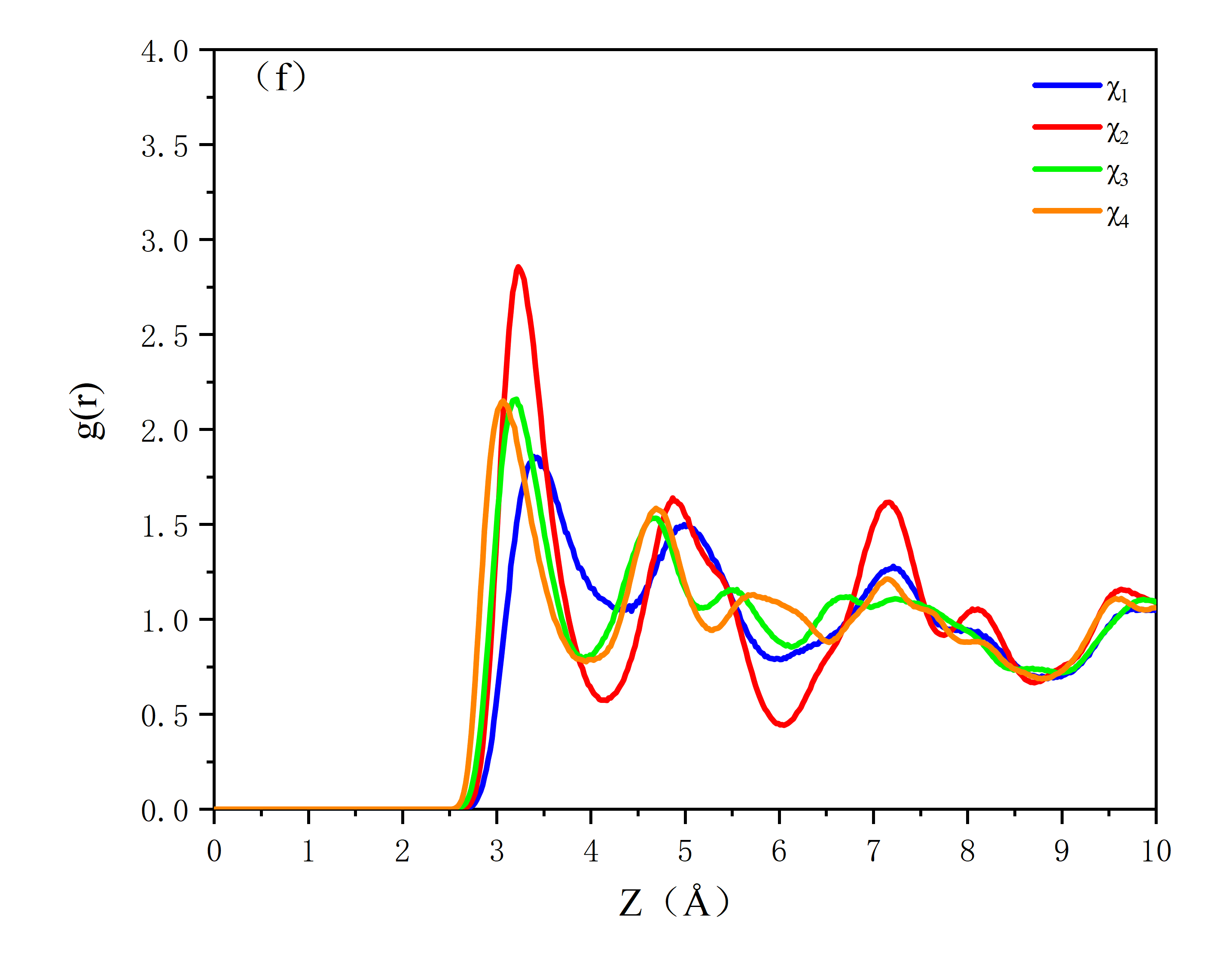
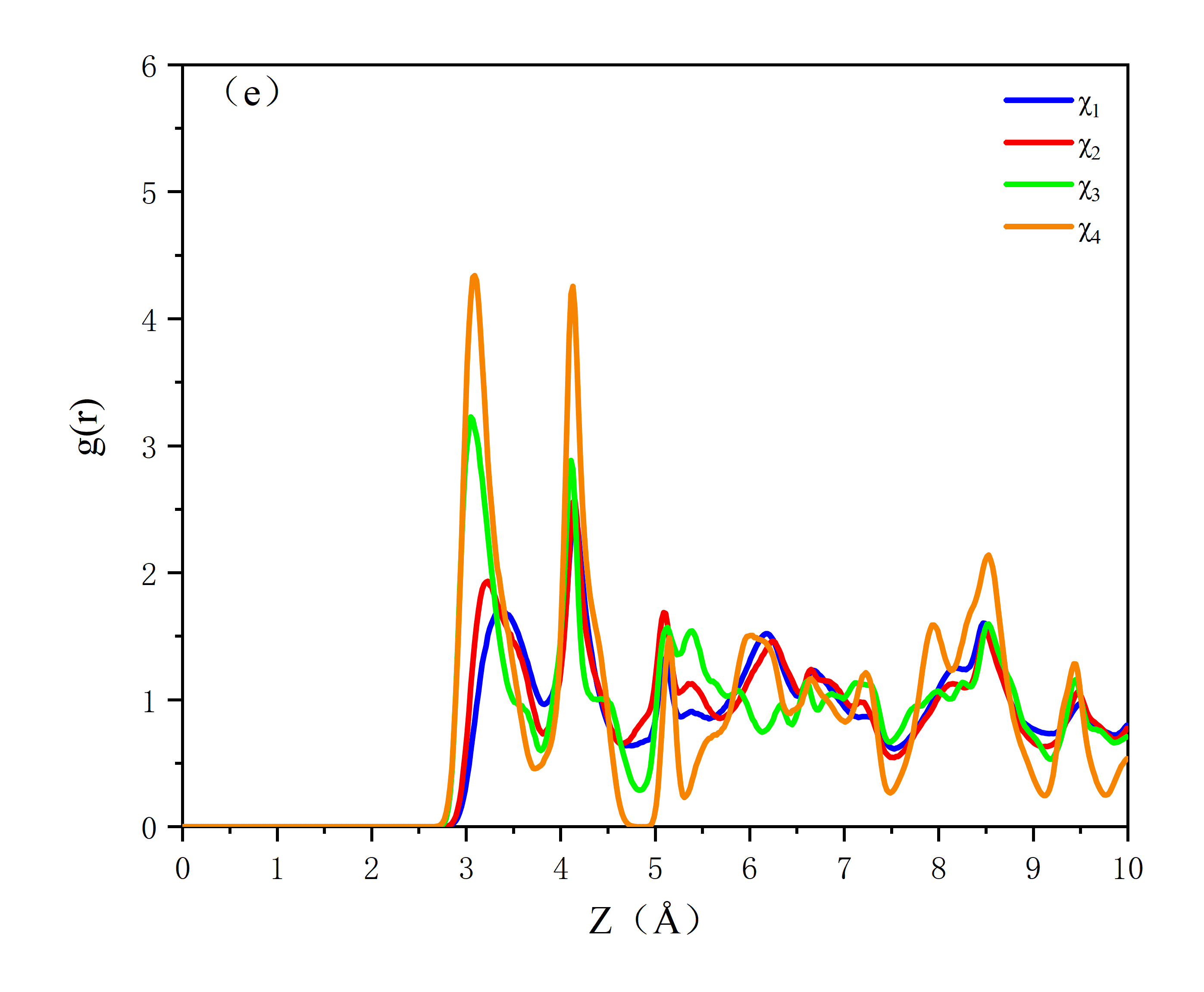
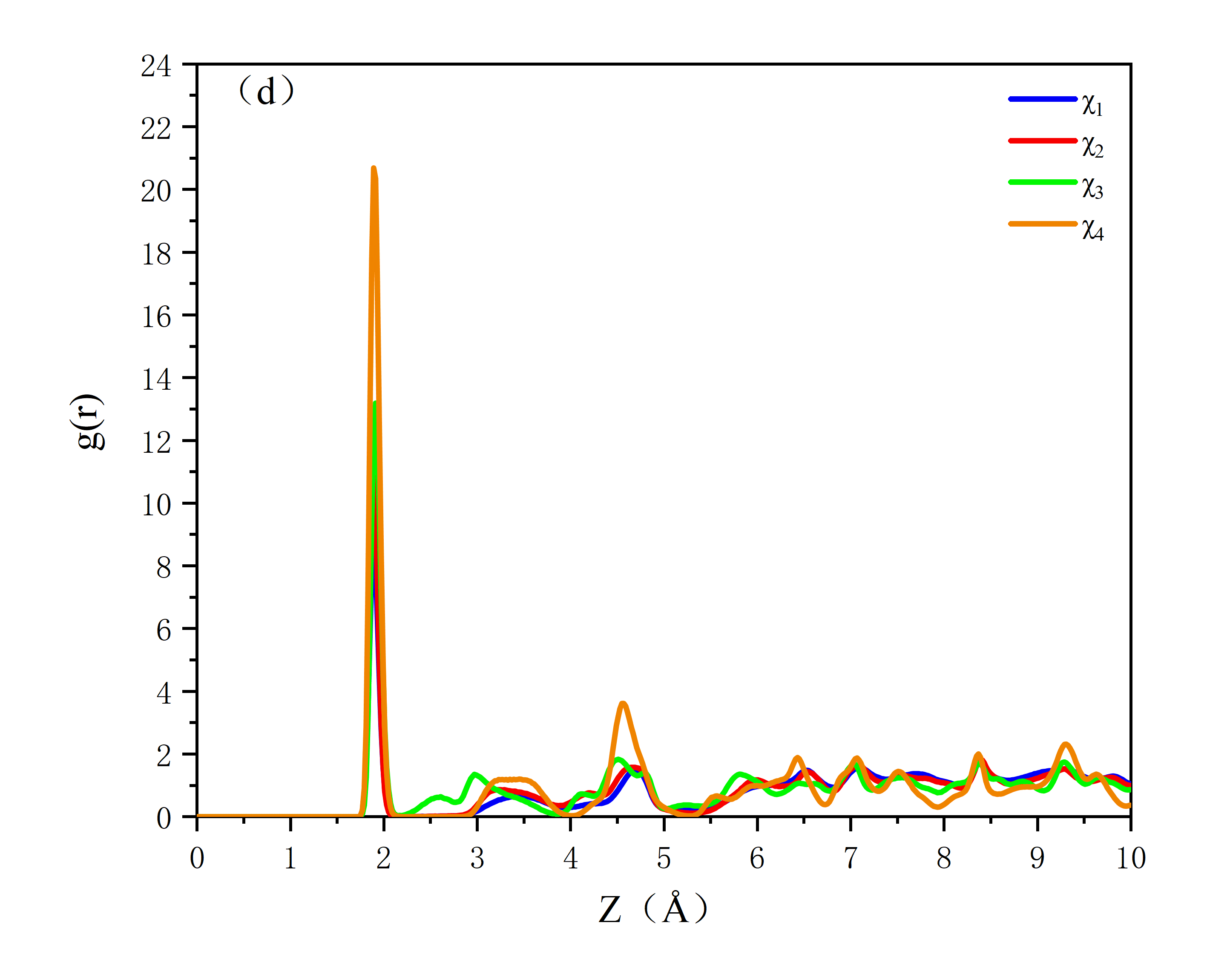
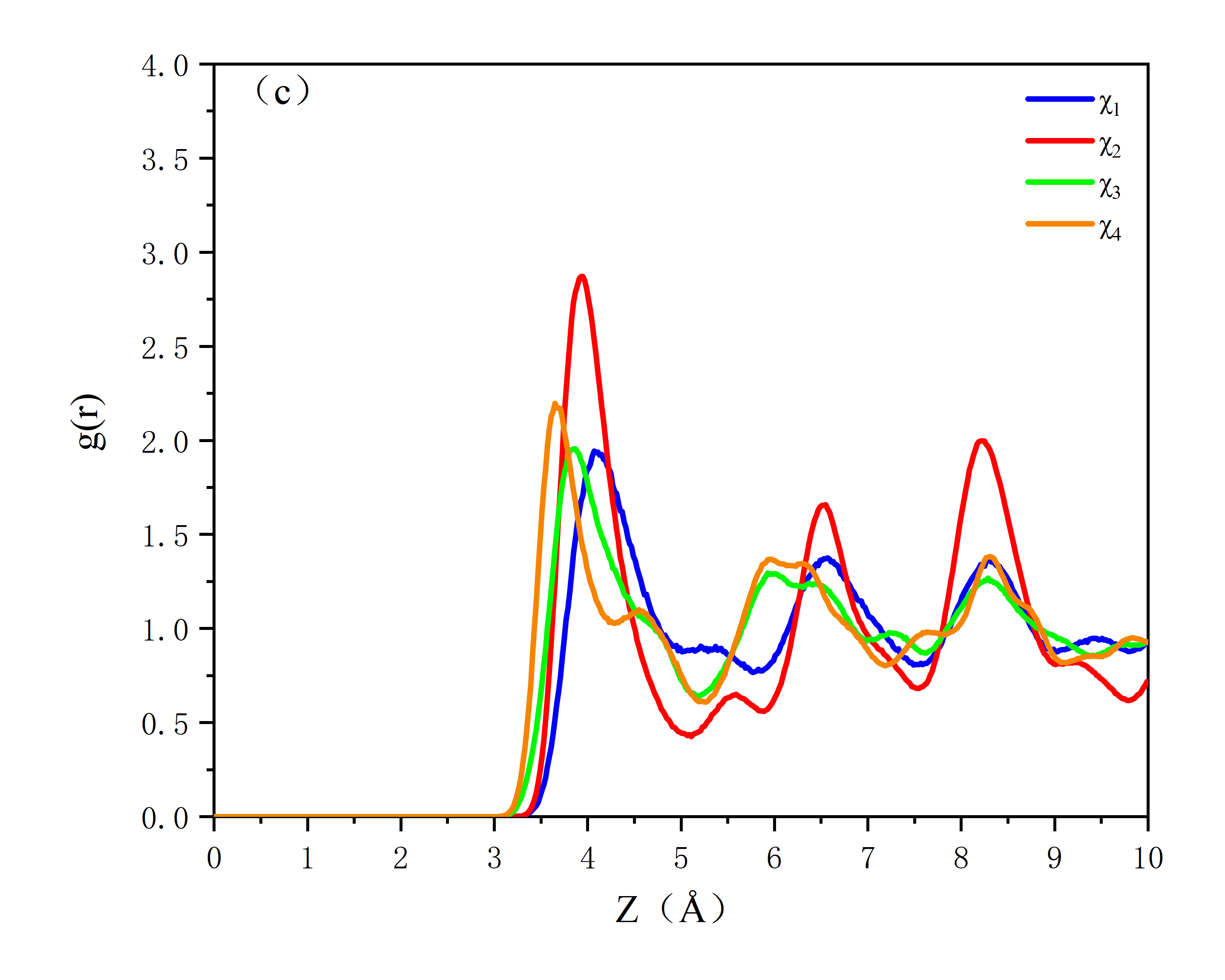
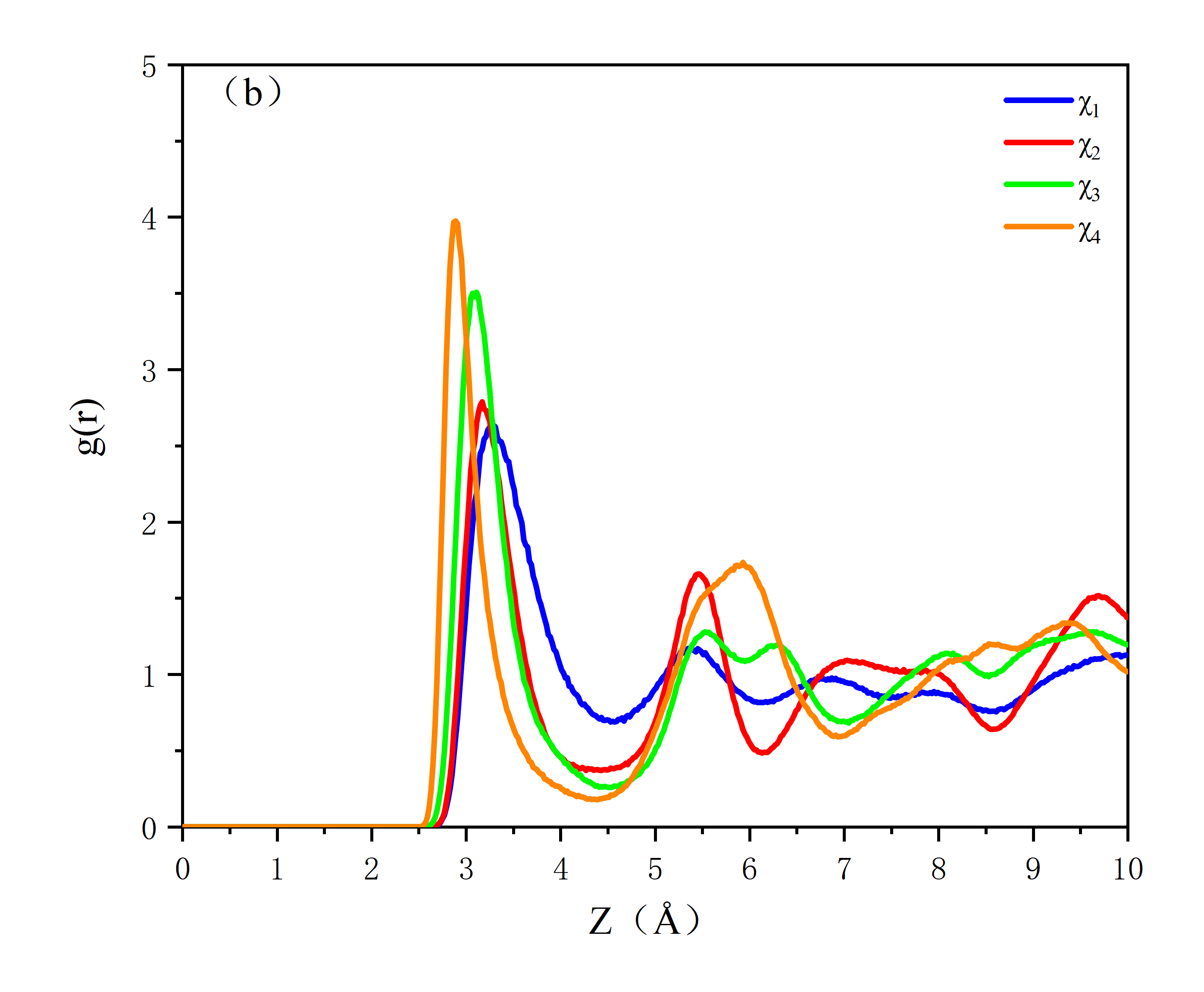
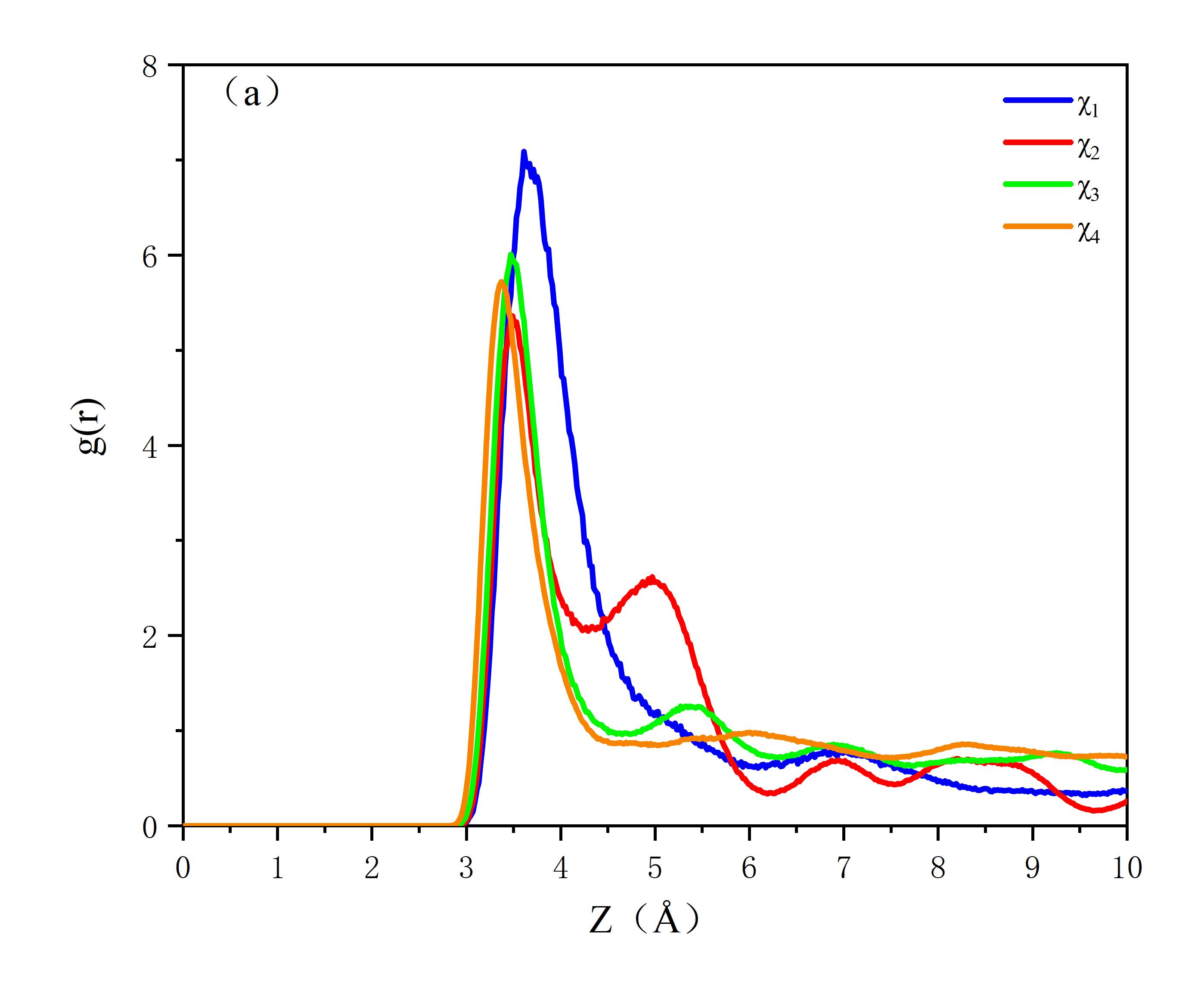
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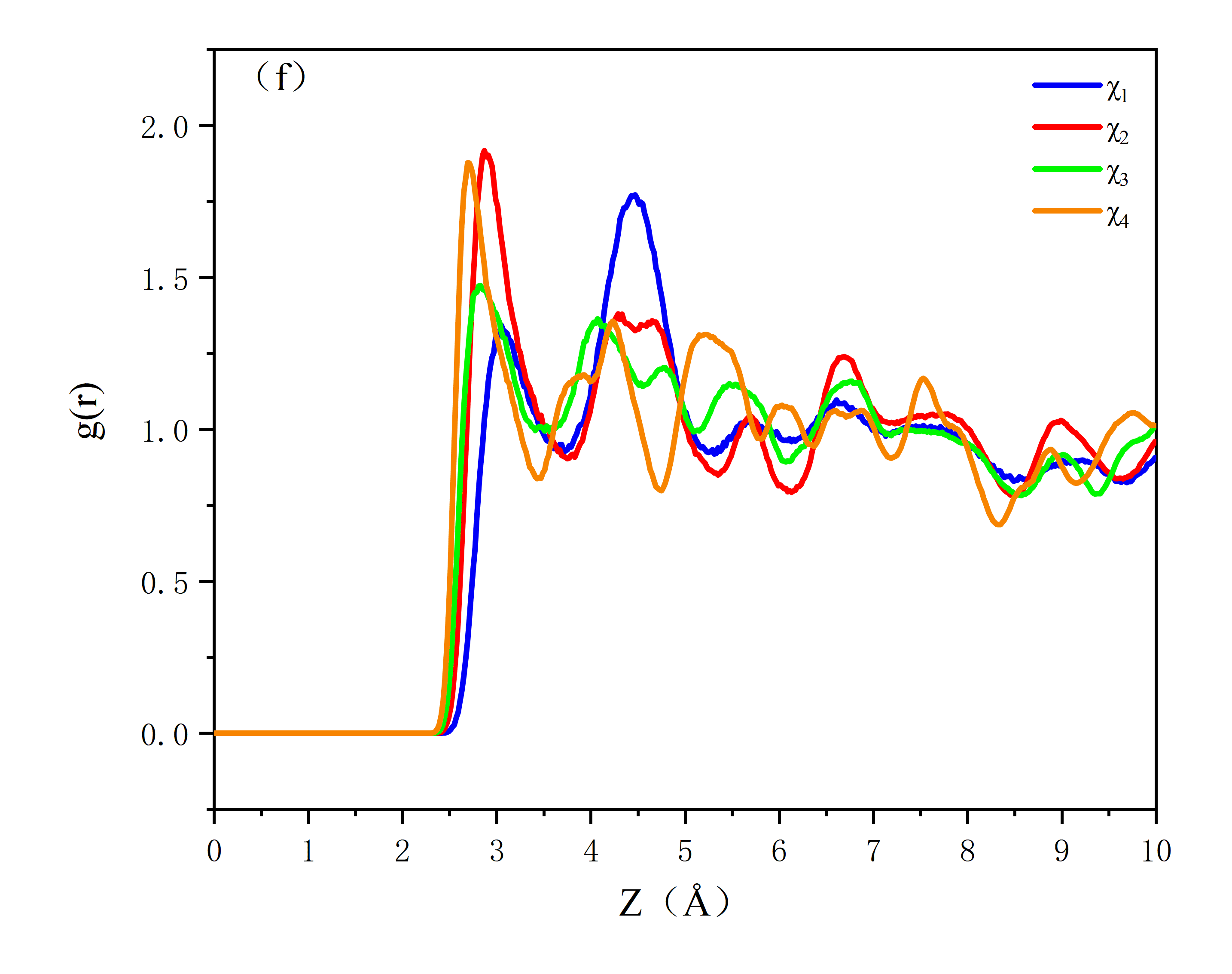
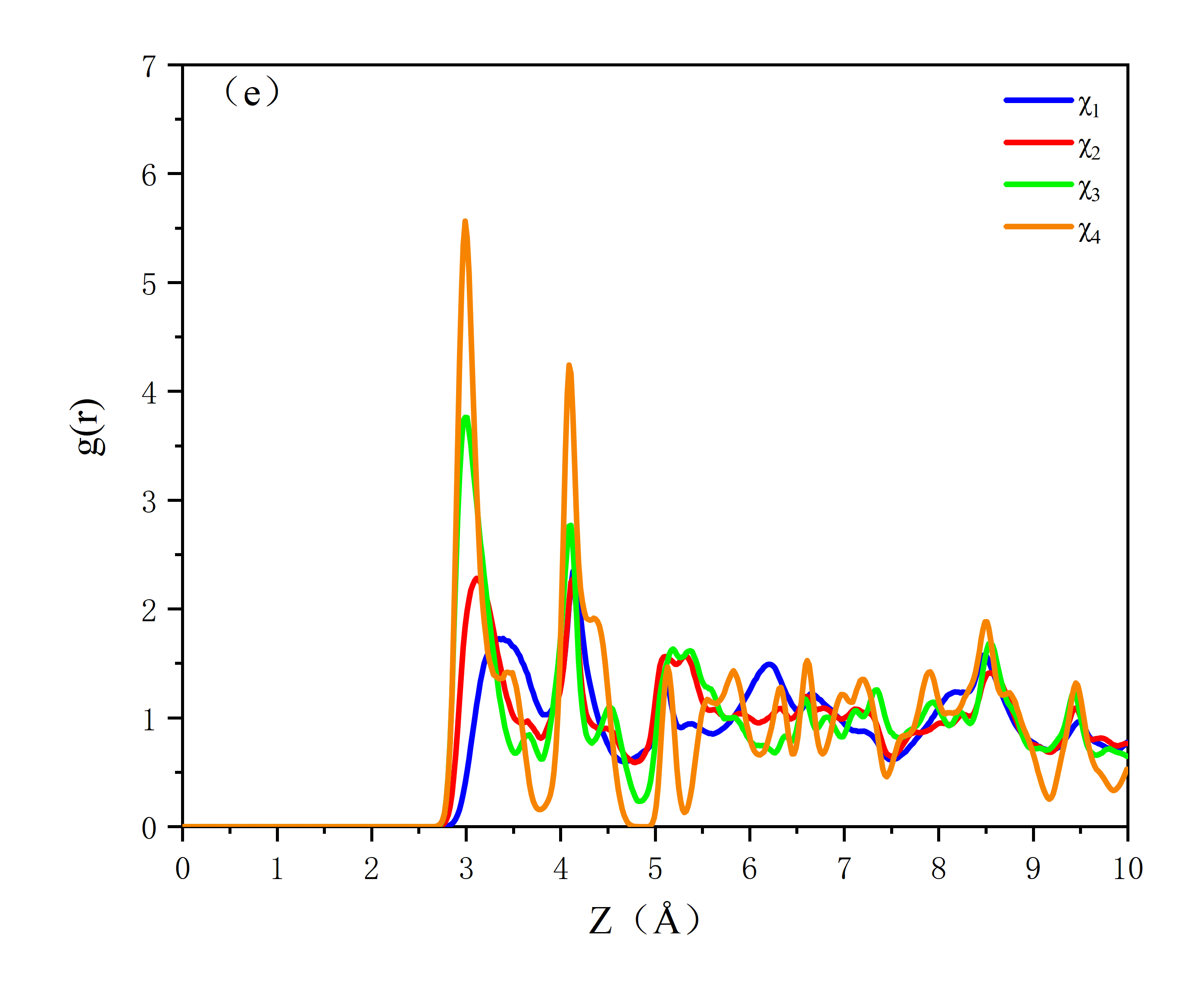
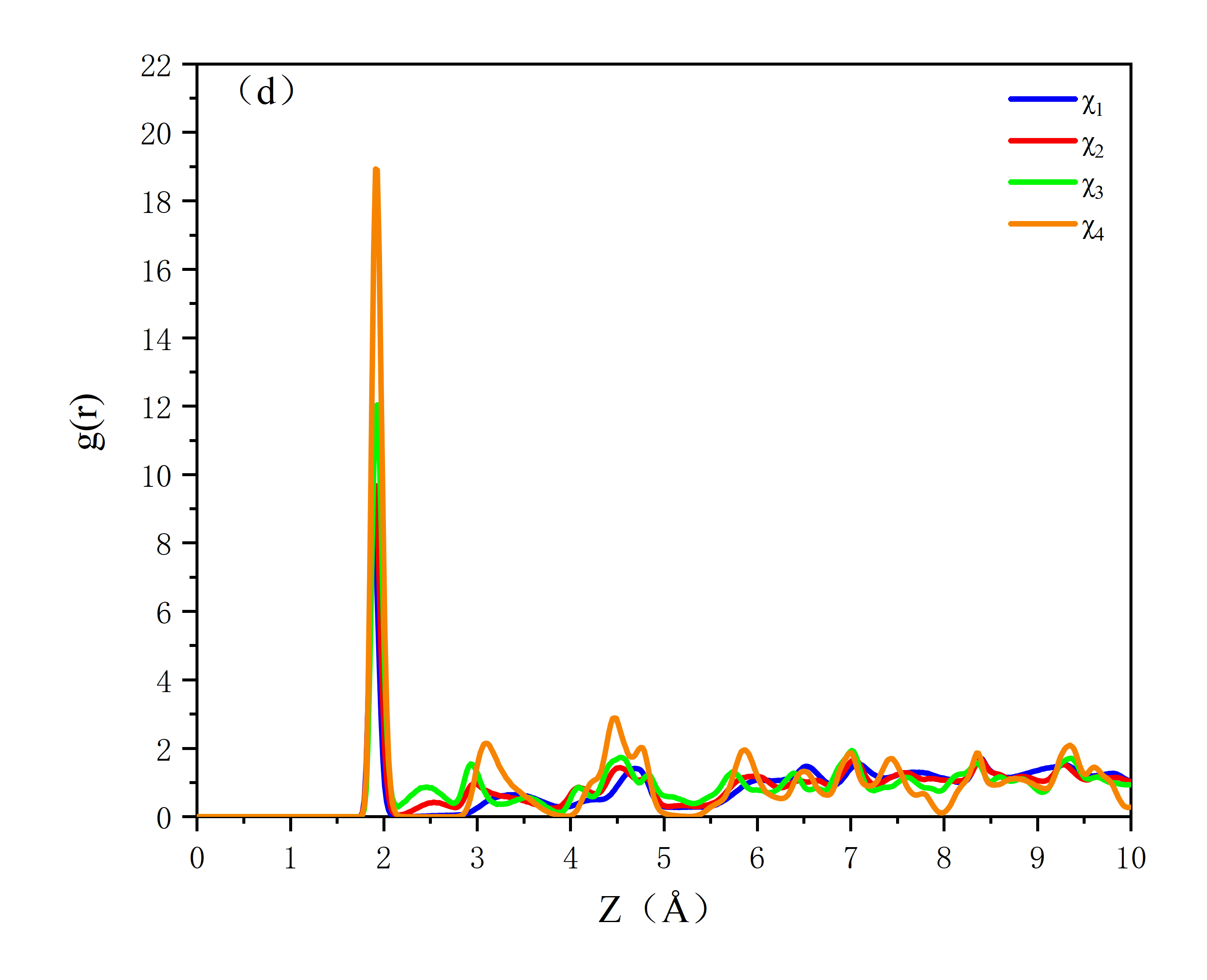
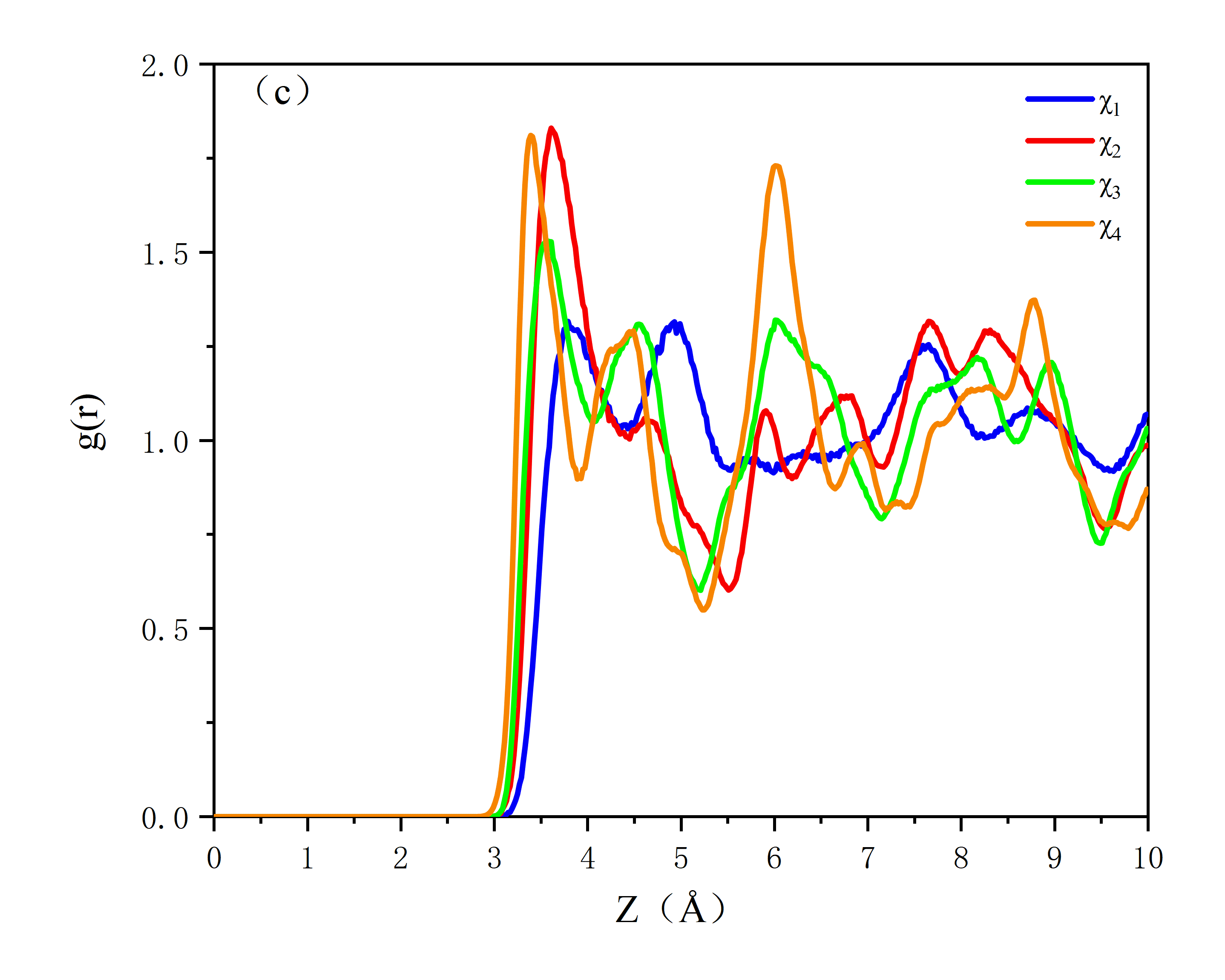
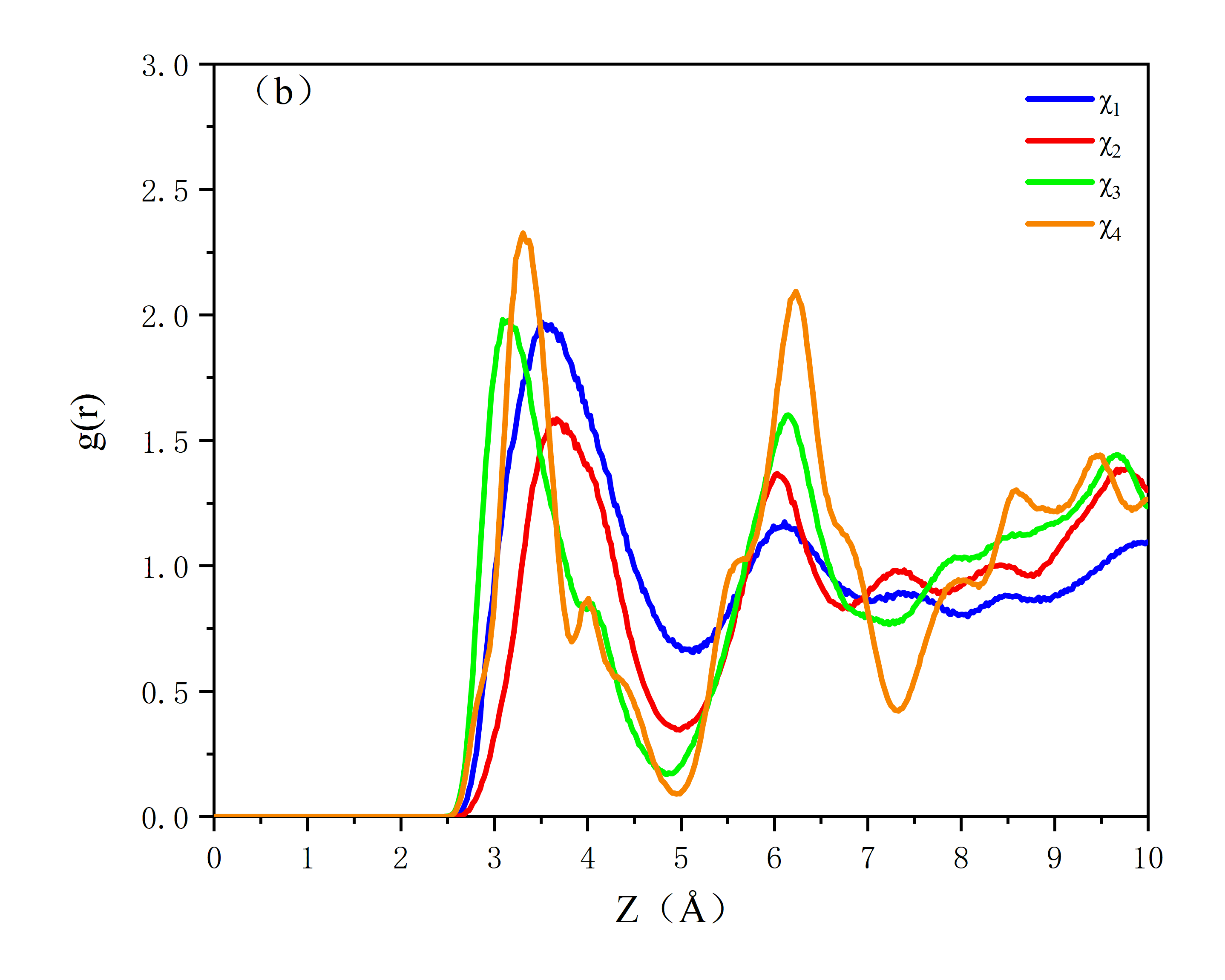
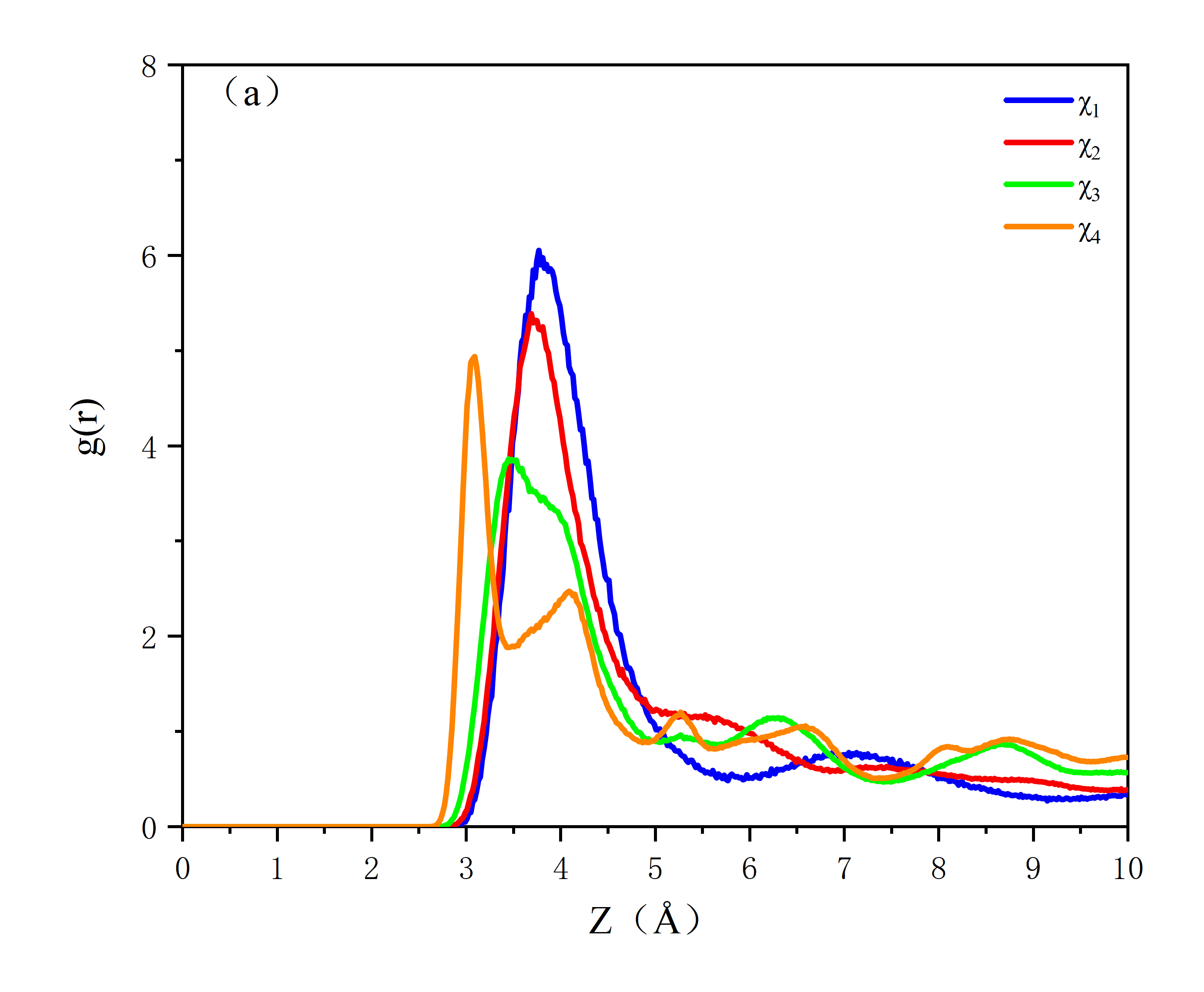
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**Figures:**



**Fig.s1** RDF patterns of H2S adsorption with different values of χi. (a) S-S; (b) S-Ow; (c) S-Si; (d) Mg-Ow; (e) Si-Ow; (f) S-Os. S: S atom in H2S; Ow: O atom in zeolitic water molecule; Si: Si atom in sepiolite; Mg: Mg atom in sepiolite; Os: O atom in structural water molecule.



**Fig.s2** RDF patterns of SO2 adsorption with different values of χi. (a) S-S; (b) S-Ow; (c) S-Si; (d) Mg-Ow; (e) Si-Ow; (f) S-Os. S: S atom in SO2; Ow: O atom in zeolitic water molecule; Si: Si atom in sepiolite; Mg: Mg atom in sepiolite; Os: O atom in structural water molecule.