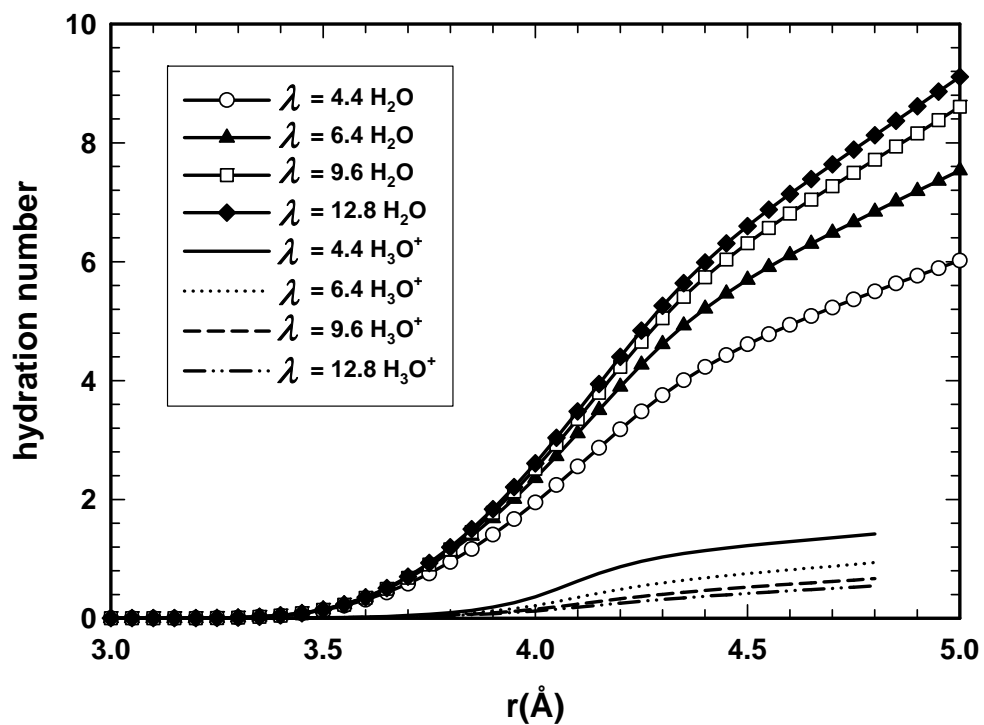
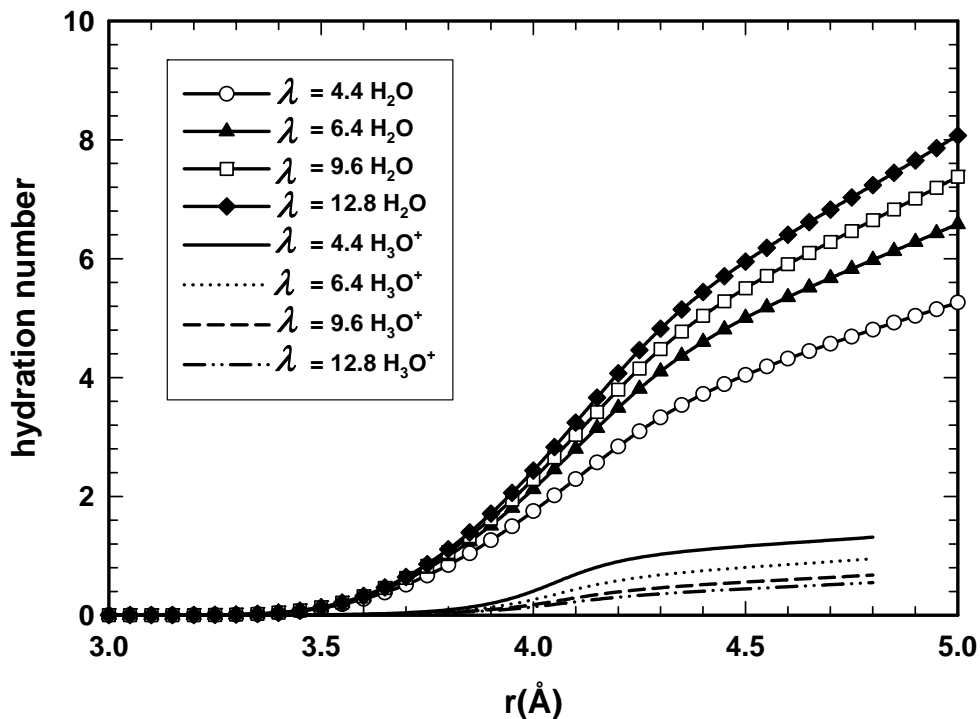


## Supporting Information



The number of water molecules (hydronium ions) around a sulfur atom of the sulfonate on the Nafion polymer. Lines with symbols: water; lines: hydronium.



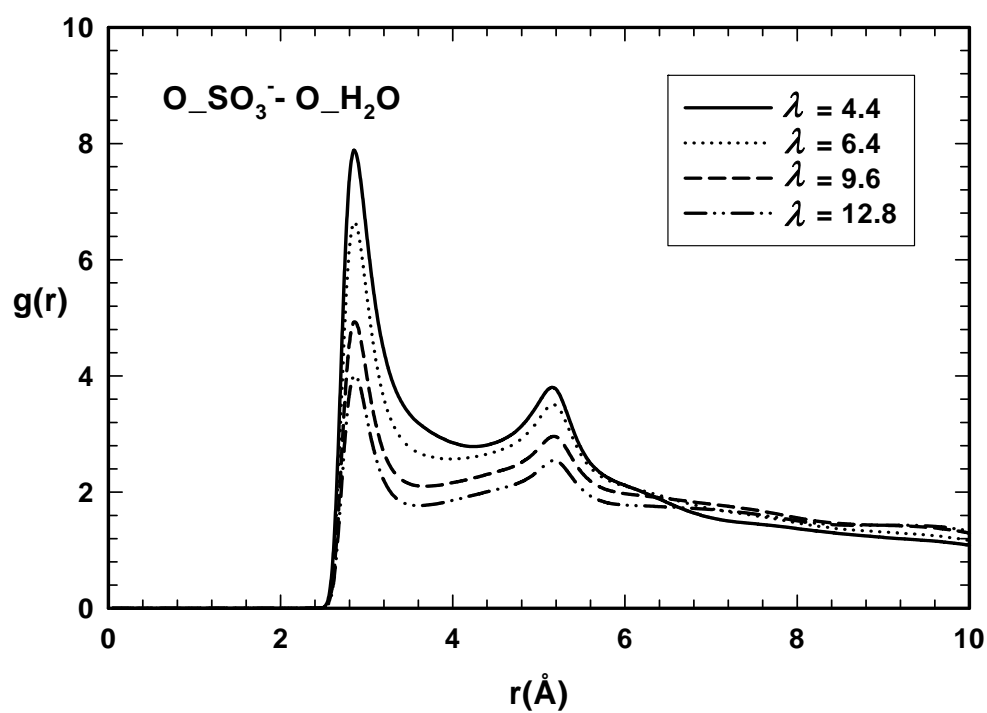
The number of water molecules (hydronium) around a sulfur atom of the sulfonate on SSC-PFSA. Lines with symbols: water; lines: hydronium ion.

Hydration number around various atomic groups of Nafion

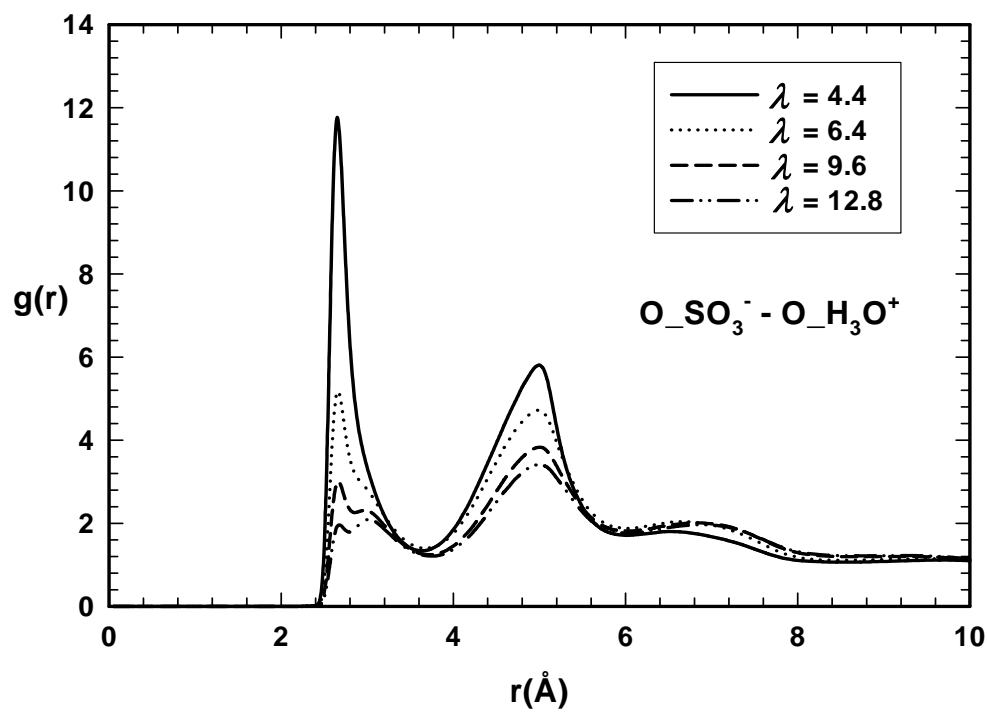
atomic types	distance	hydration number for different water content			
		$\lambda = 4.4$	$\lambda = 6.4$	$\lambda = 9.6$	$\lambda = 12.8$
sulfur-O of H <sub>2</sub> O	0-5.0 Å	6.02	7.53	8.61	9.11
sulfur-O of H <sub>3</sub> O <sup>+</sup>	0-4.8 Å	1.41	0.93	0.67	0.54
O of SO <sub>3</sub> <sup>-</sup> -O of H <sub>2</sub> O	0-4.0 Å	2.58	3.19	3.58	3.77
O of SO <sub>3</sub> <sup>-</sup> -O of H <sub>3</sub> O <sup>+</sup>	0-3.5 Å	0.43	0.27	0.19	0.15
O of H <sub>3</sub> O <sup>+</sup> -O of H <sub>2</sub> O	0-3.2 Å	2.56	3.08	3.37	3.49

Hydration number around various atomic groups of SSC-PFSA

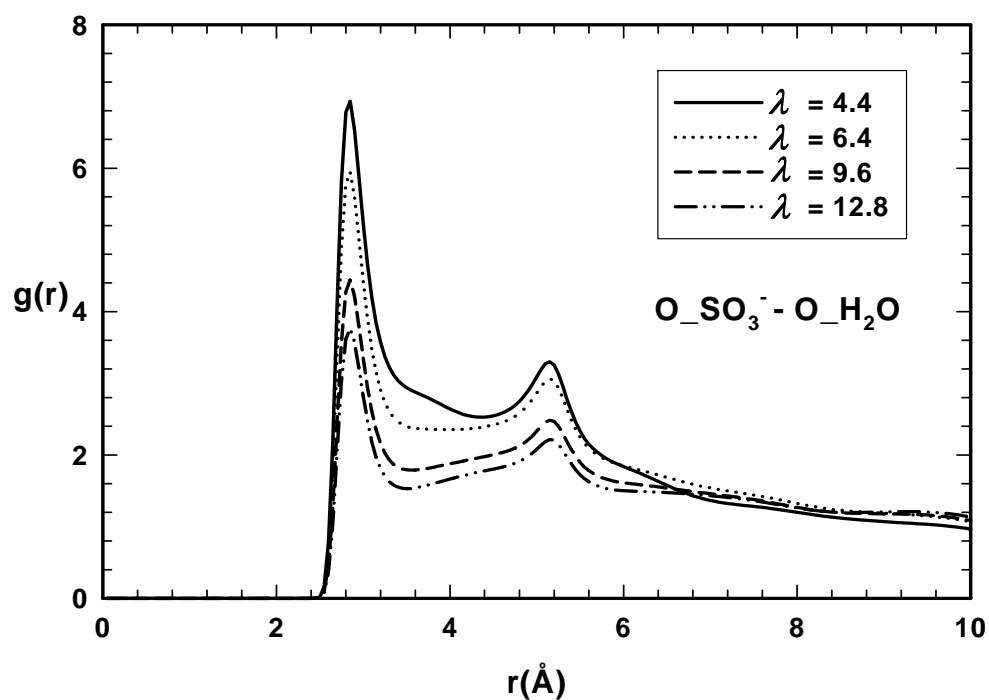
atomic types	distance	hydration number for different water content			
		$\lambda = 4.4$	$\lambda = 6.4$	$\lambda = 9.6$	$\lambda = 12.8$
sulfur-O of H <sub>2</sub> O	0-5.0 Å	5.26	6.58	7.38	8.07
sulfur-O of H <sub>3</sub> O <sup>+</sup>	0-4.8 Å	1.31	0.95	0.68	0.55
O of SO <sub>3</sub> <sup>-</sup> -O of H <sub>2</sub> O	0-4.0 Å	2.26	2.78	3.08	3.34
O of SO <sub>3</sub> <sup>-</sup> -O of H <sub>3</sub> O <sup>+</sup>	0-3.5 Å	0.40	0.28	0.20	0.15
O of H <sub>3</sub> O <sup>+</sup> -O of H <sub>2</sub> O	0-3.2 Å	2.10	2.56	2.86	3.01



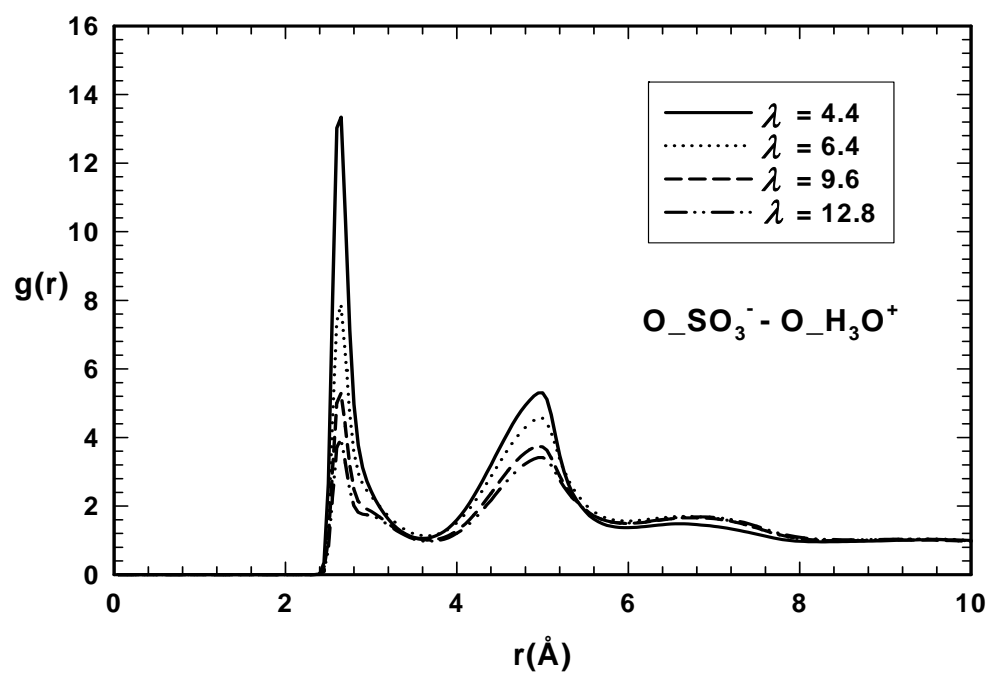
The pair correlation function between the oxygen of the sulfonate group on Nafion and oxygen of water molecules.



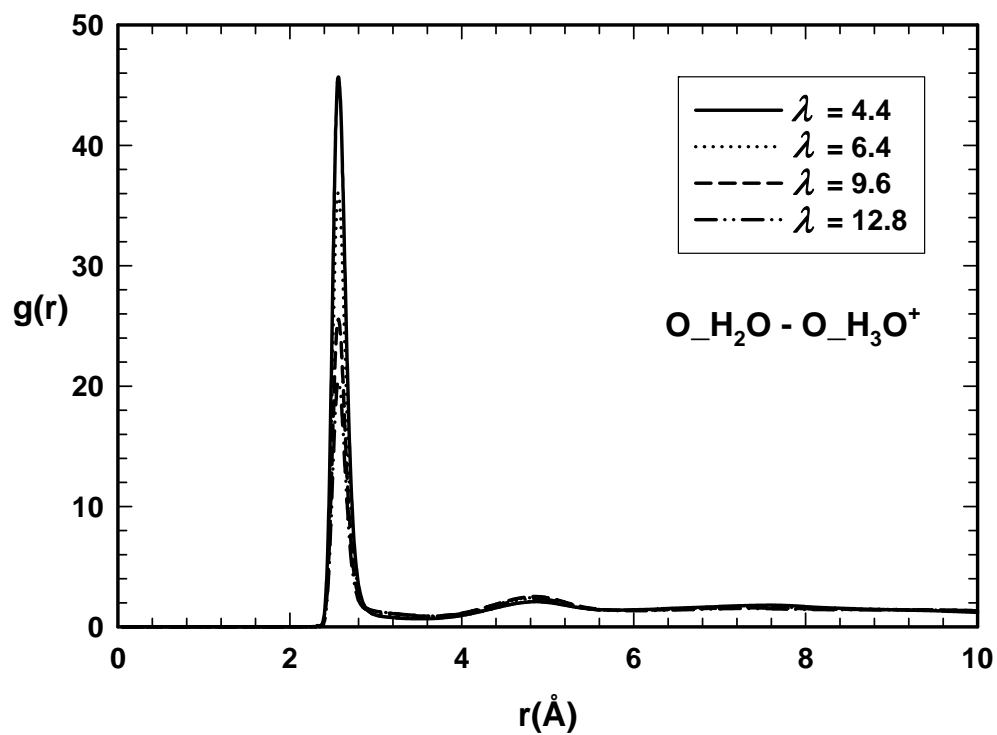
The pair correlation function between the oxygen of the sulfonate group on Nafion and oxygen of hydronium ion.



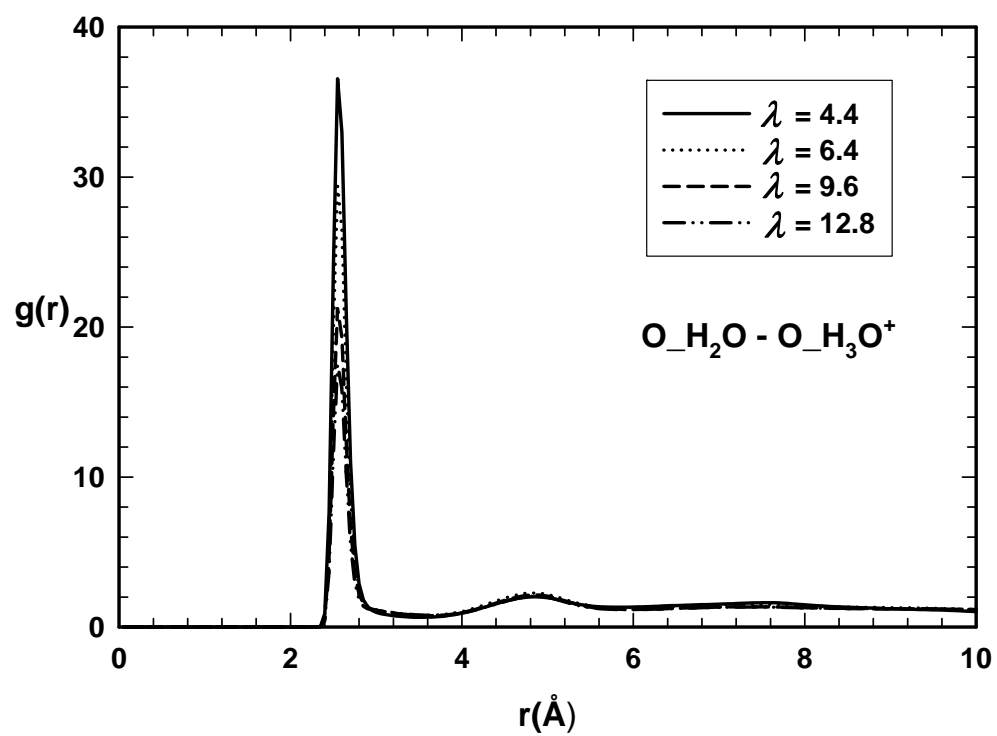
The pair correlation function between the oxygen of the sulfonate group on SSC PFSA and oxygen of water molecules.



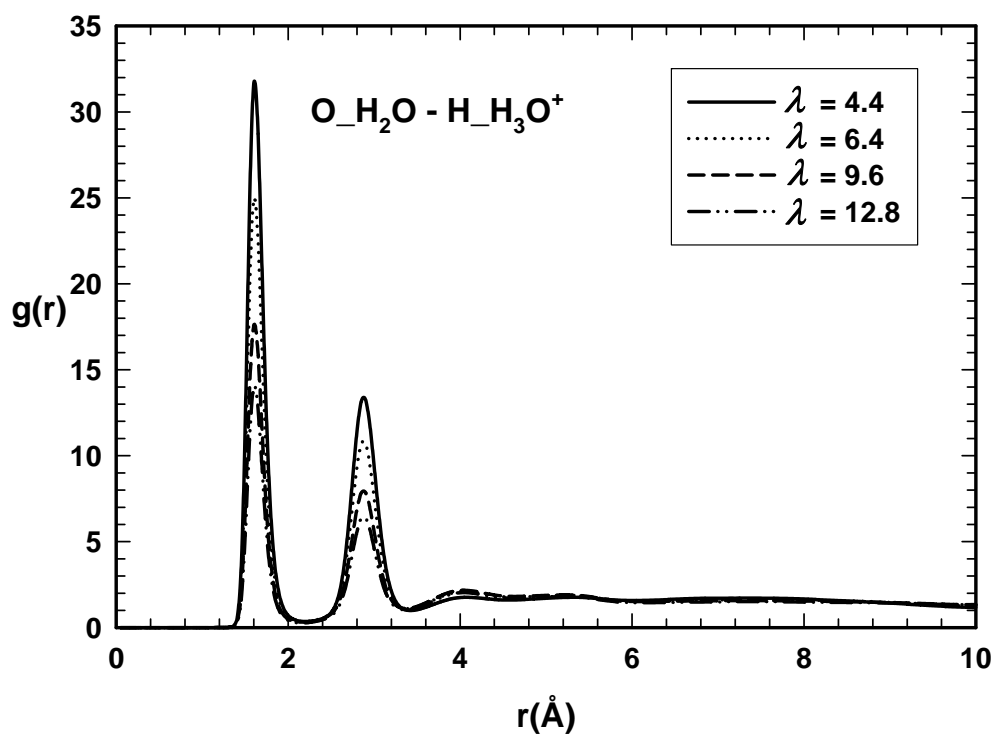
The pair correlation function between the oxygen of the sulfonate group on SSC PFSA and oxygen of hydronium ion.



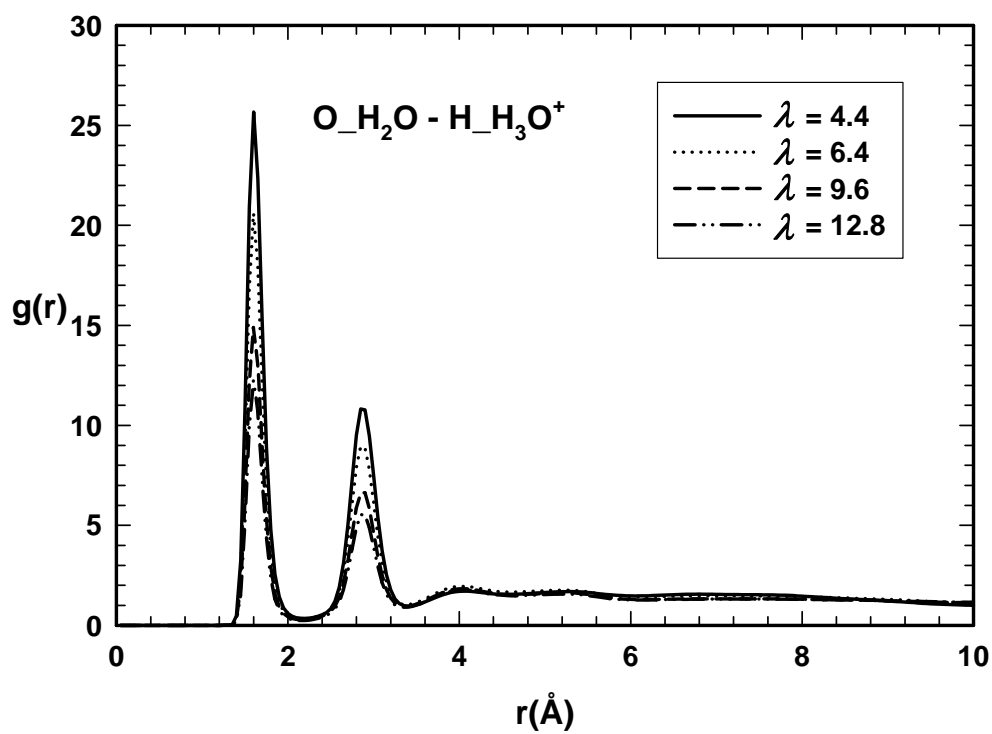
The PCF for the oxygen of water and the oxygen of hydronium ion in hydrated Nafion.



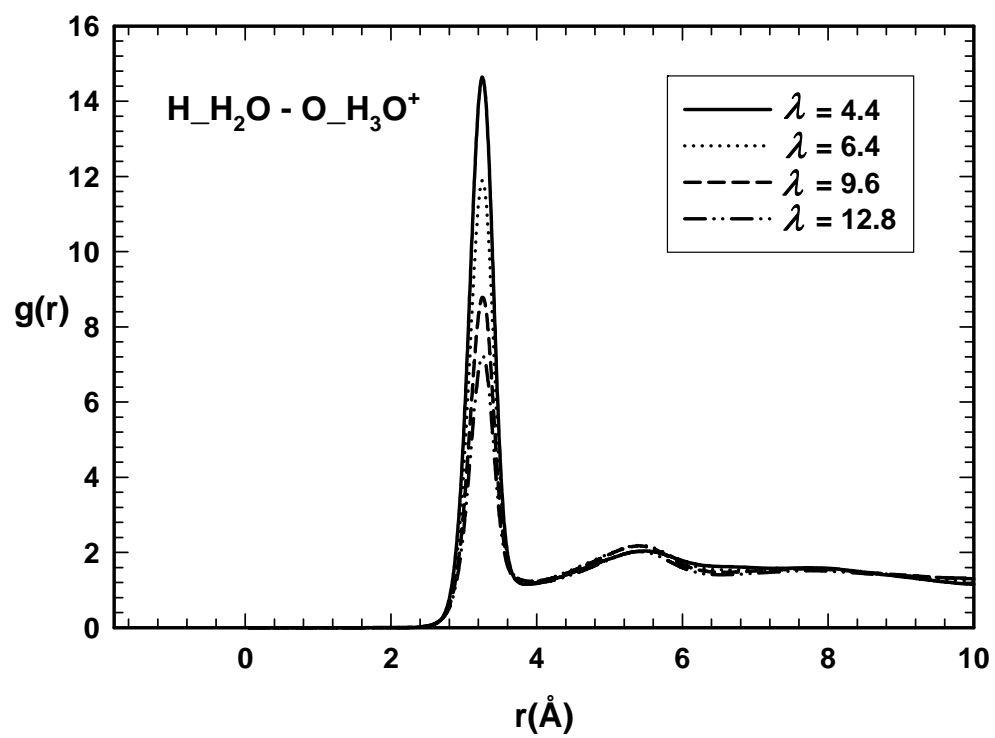
The PCF for the oxygen of water and the oxygen of hydronium ion in hydrated SSC PFSA



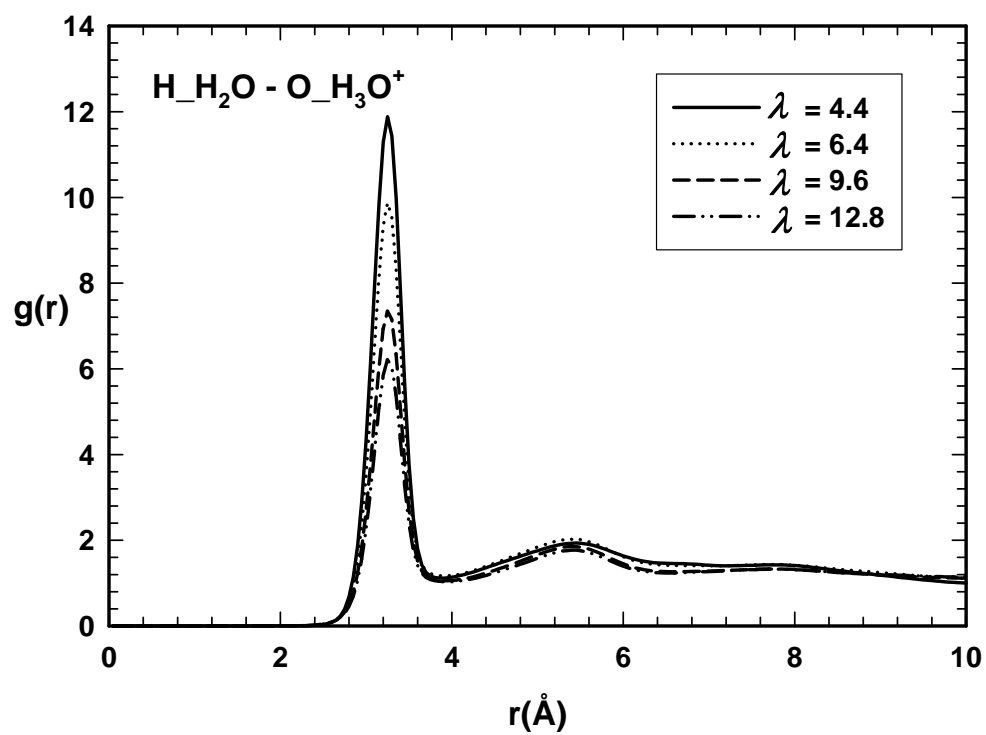
The PCF for the oxygen of water and the hydrogen of hydronium ion in hydrated Nafion.



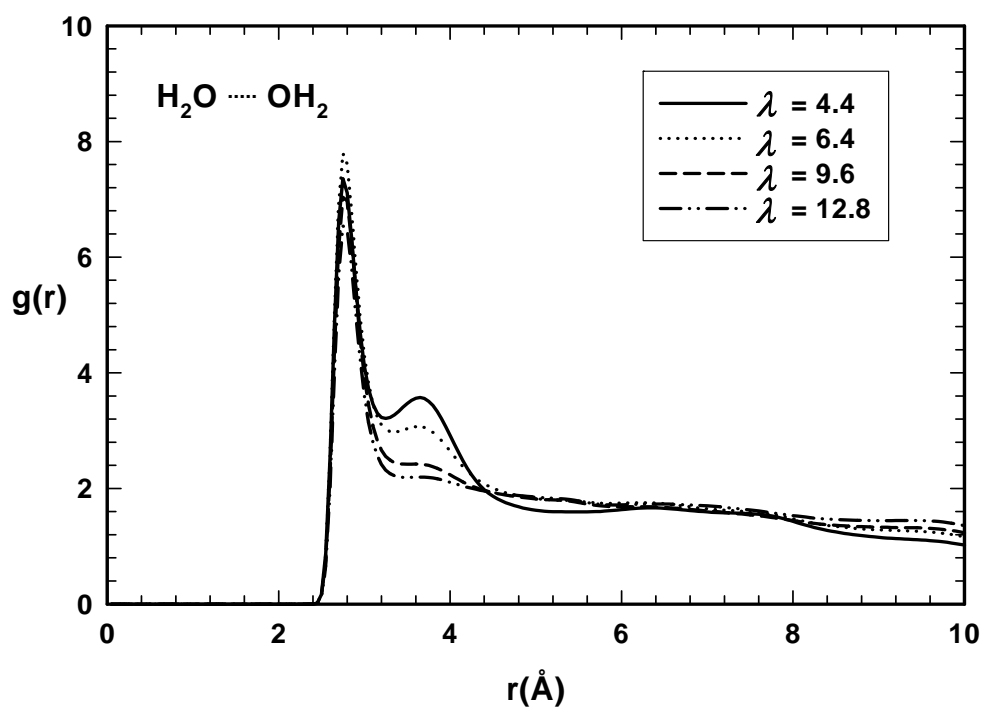
The PCF for the oxygen of water and the hydrogen of hydronium ion in hydrated SSC PFSA.



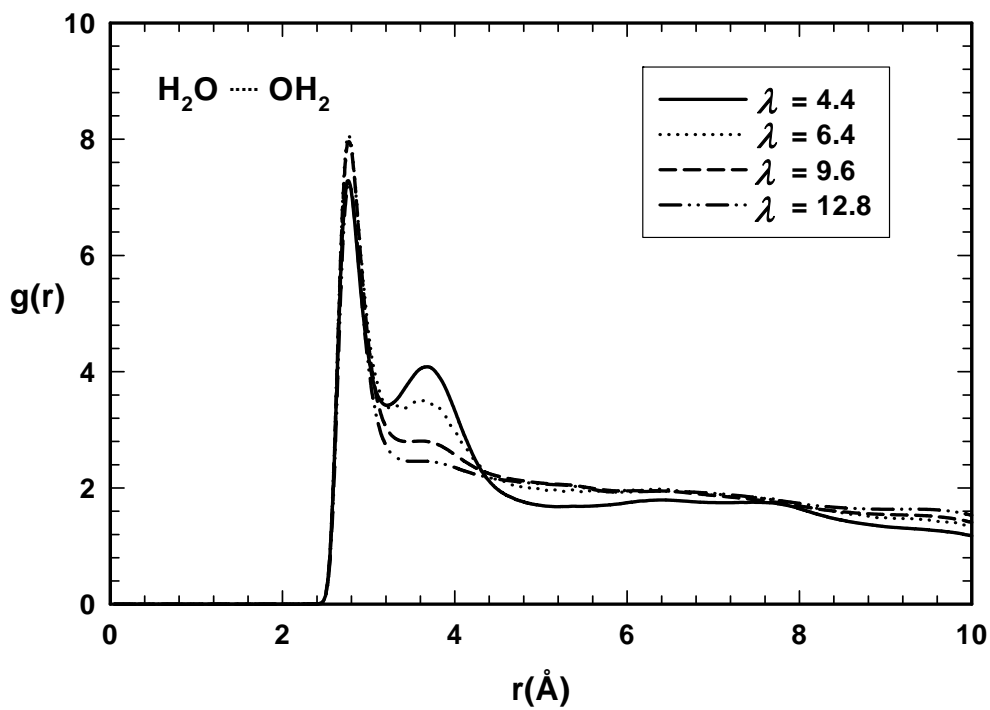
The PCF for the hydrogen of water and the oxygen of hydronium ion in hydrated Nafion.



PCF for the hydrogen of water and the oxygen of hydronium ion in hydrated SSC PFSA.



Water-water (as represented by oxygen of water molecules) PCF for SSC PFSA.



Water-water (as represented by oxygen of water molecules) PCF for Nafion.