## Supplementary Materials: Understanding Cationic Polymer Adsorption on Mineral Surfaces: Kaolinite in Cement Aggregates

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**Table S1.** Electronic structure of the norm-conserving pseudopotentials (GGA-PBE where available).

Element	Configuration
Al	$3s^23p^1$
С	$3s^23p^1 \ 2s^22p^2$
Н	$1s^1$
N	$2s^22p^3$
O	$2s^22p^4$
Si	$2s^{2}2p^{3}$ $2s^{2}2p^{4}$ $3s^{2}3p^{2}$ $3s^{2}3p^{5}$
Cl	$3s^23p^5$



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