Supporting Information:

First-Principles Modeling of Transport Mechanisms in Carbonate-Hydroxide Electrolytes

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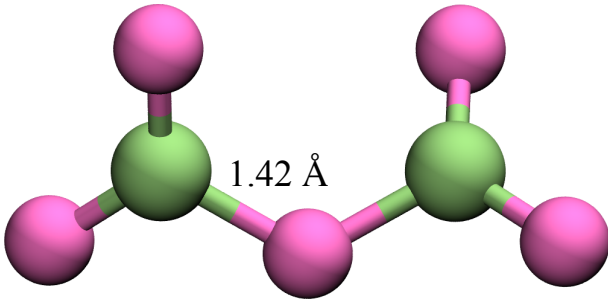

Figure S1: Gas phase optimized geometry of pyrocarbonate anion at the MP2/aug-cc-pVQZ level of theory. Color scheme: carbon - lime, oxygen - mauve.

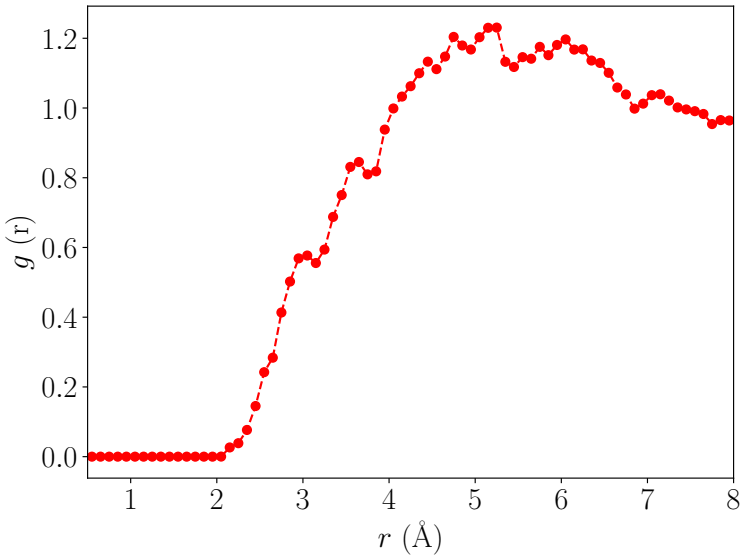

Figure S2: Radial distribution functions between the carbon atom of CO_2 and oxygen atoms of CO_3^{2-} below 1 ps timescale.

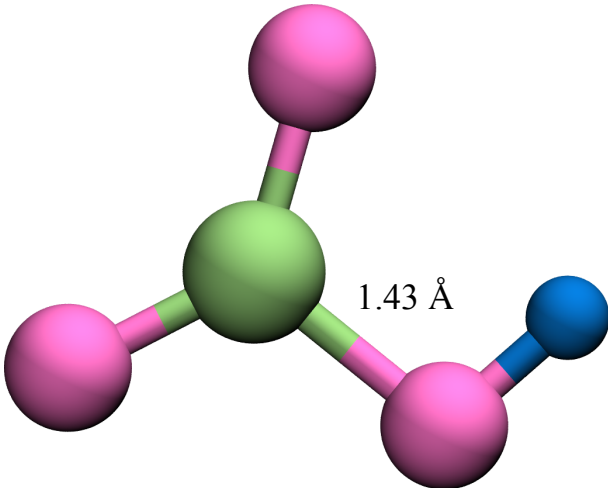

Figure S3: Gas phase optimized geometry of bicarbonate anion at the MP2/aug-cc-pVQZ level of theory. Color scheme: carbon - lime, oxygen - mauve, hydrogen - blue.

Table S1: Exponential fit parameters to lifetime distributions plotted in Figure 10 of the main text.

Species	a	b (ps^{-1})
CO_3^{2-}	748	1.40
OH^-	204	1.44
CO_2	25.8	2.09
$C_2O_5^{2-}$	48.2	2.52
HCO_3^-	152	5.25
H_2O	117	3.37

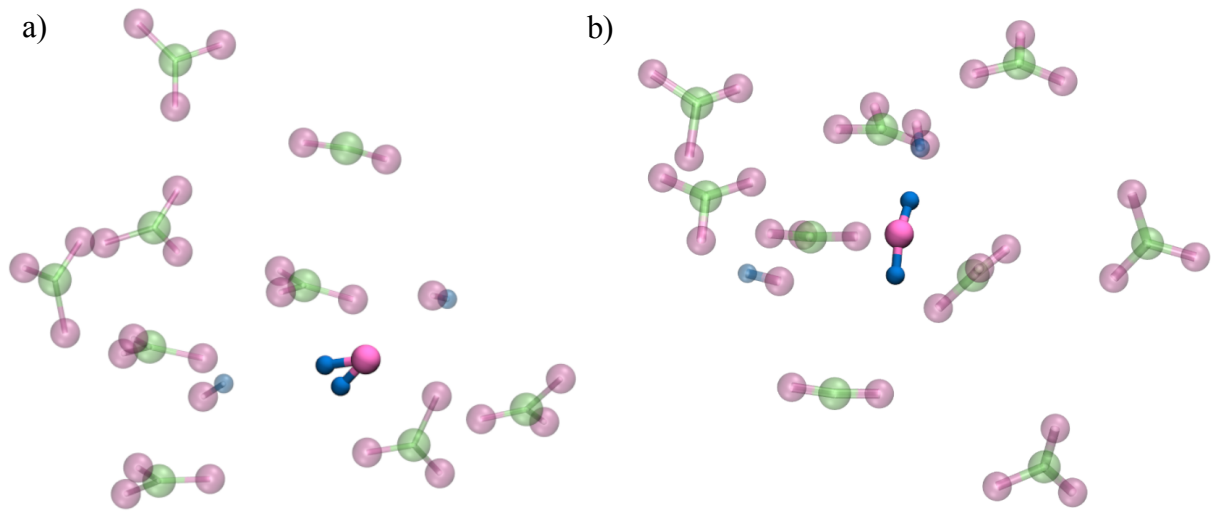

Figure S4: AIMD simulation snapshots representing two extreme geometries in H_2O – a) HOH angle 22° and b) HOH angle 166°. Color scheme: C – lime; O – mauve; H – blue. Rest of the atoms are shown as transparent background for clarity.