Supporting Information

Bridging Electron and Nuclear Motions in Chemical Reactions through Electrostatic Forces from Reactive Orbitals

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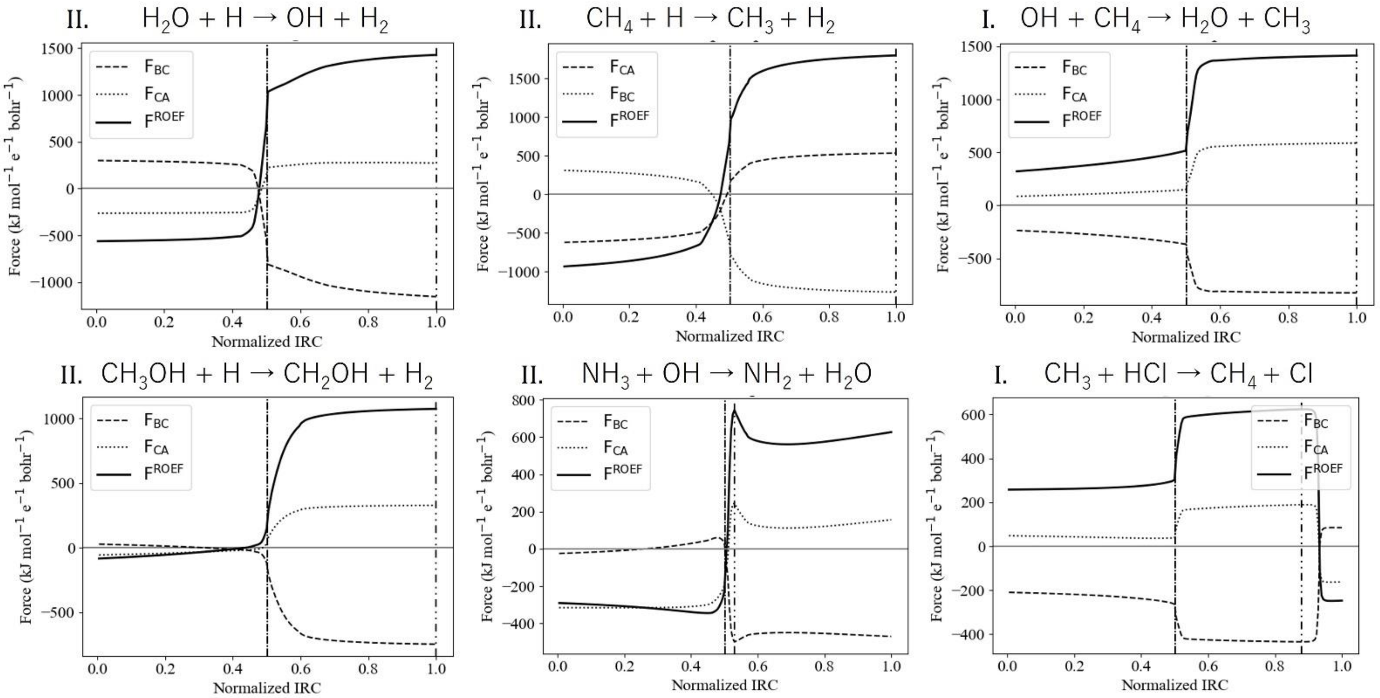
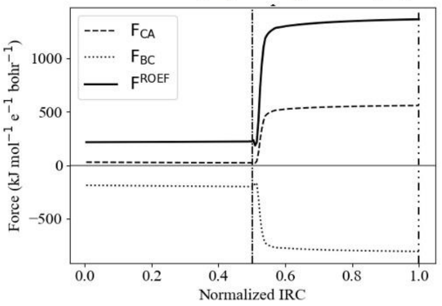
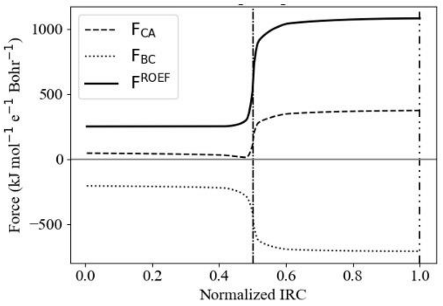
Figure S1. Variations in reactive orbital-based electrostatic force (ROEF) vectors along the B-C and C-A bond directions, represented by F_{BC} (red curves) and F_{CA} (blue curves), against the normalized intrinsic reaction coordinates (IRCs). These ROEF vector variations correspond to characteristic atom transfer reactions and are categorized into four types: I. Continuous forward ROEFs throughout the reaction, II. Sudden reaction-forward ROEFs just before the transition states (TSs), III. Forward ROEFs persisting until reaching the TSs followed by backward ROEFs, and IV. Backward ROEFs after the TSs, for forward processes. The variations are shown only for representative reactions of these types. ROEFs are derived from occupied reactive orbitals, as described in Eq. (8). The definitions for the vectors of F_{BC} and F_{CA} are detailed in Fig. 1(b). Green dotted lines mark the TS locations, while orange dotted lines indicate points where the combined ROEF values directed towards the reaction, F_{CA} - F_{BC}, reach their maximum. In parentheses attaching reaction formulae, the spin states of the reactive molecular orbitals that give larger maximum ROEF values are indicated.



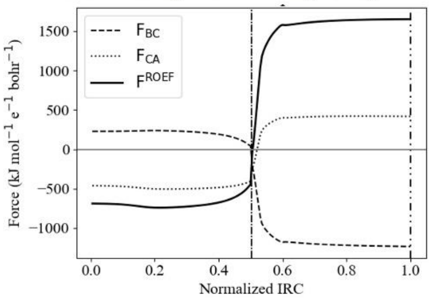
I. $OH + C_2H_6 \rightarrow H_2O + C_2H_5$



I. $CH_3 + OH \rightarrow CH_4 + O$



II. $PH_3 + H \rightarrow PH_2 + H_2$



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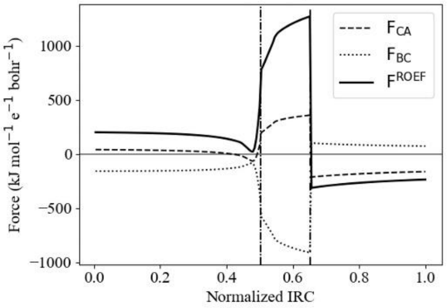
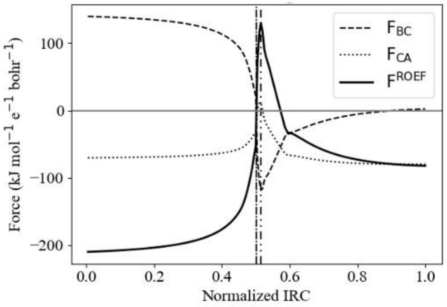
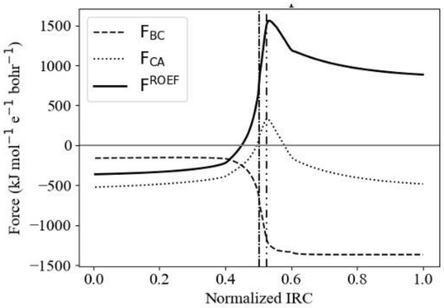


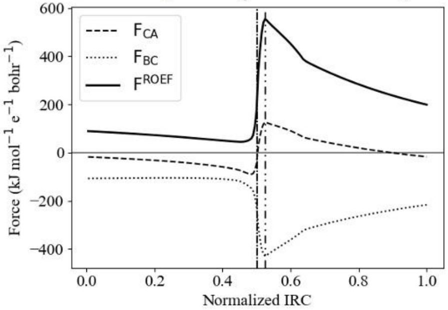
II. $H_2S + H \rightarrow SH + H_2$



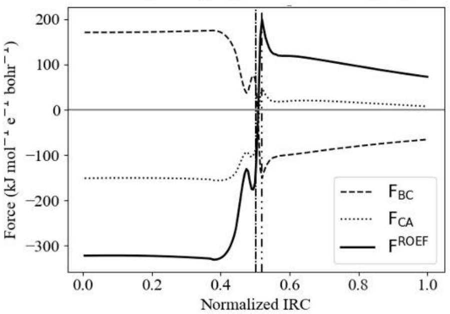
II. $HCl + O \rightarrow Cl + OH$



I. $NH_2 + CH_3 \rightarrow NH + CH_4$



II. $NH_2 + C_2H_5 \rightarrow NH + C_2H_6$



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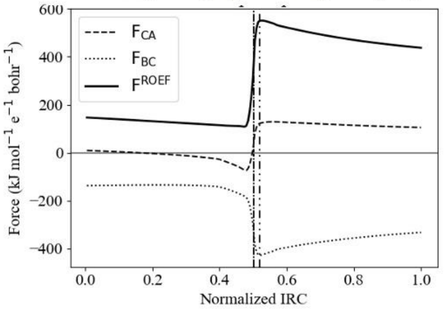
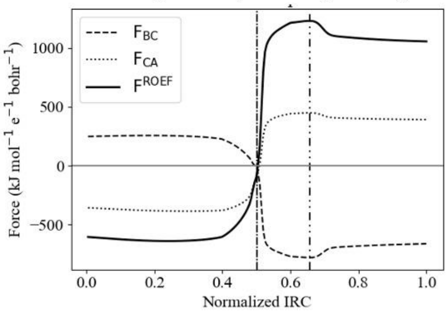
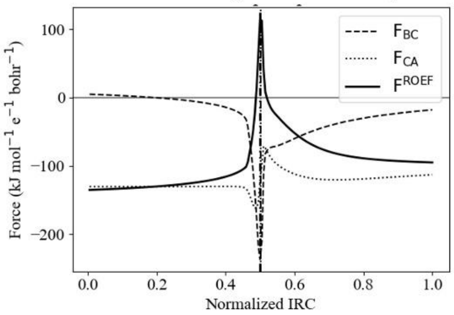


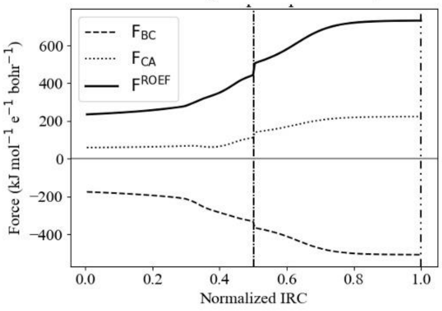
II. $NH_2 + CH_4 \rightarrow NH_3 + CH_3$

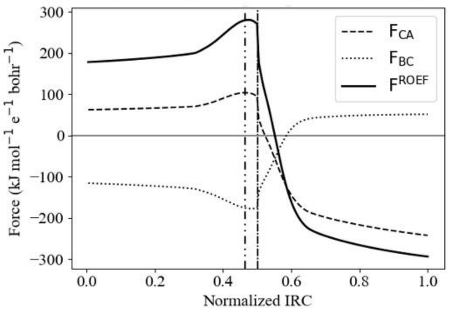


II. $H + FCH_3 \rightarrow HF + CH_3$

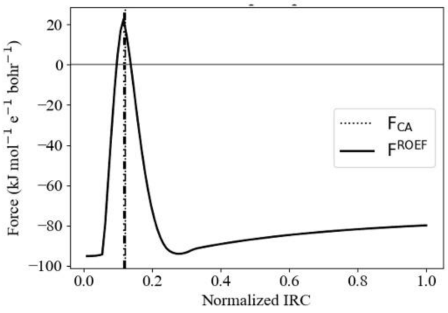


I. $Cl^- + CH_3F \rightarrow F^- + CH_3Cl$

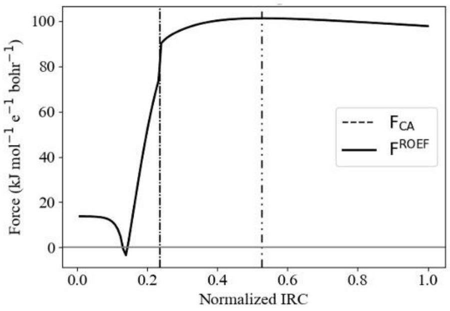




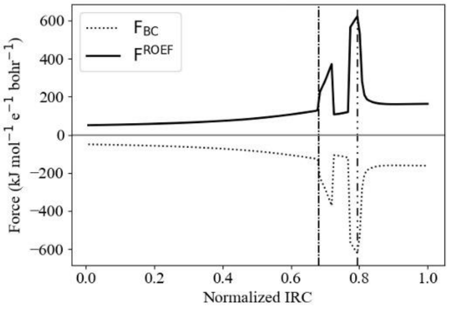
III. $OHCH_3 + F^- \rightarrow OH^- + CH_3F$



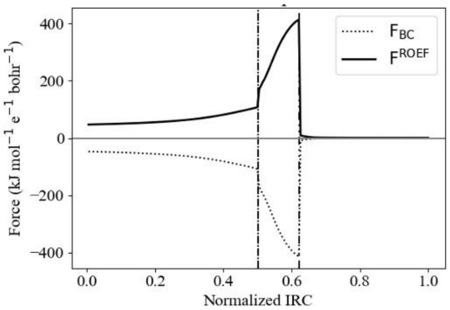
III. $HN_2 \rightarrow H + N_2$



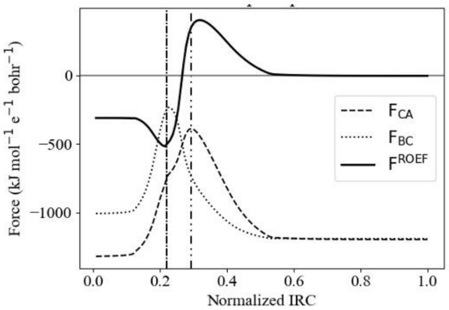
I. $HCO \rightarrow CO + H$



I. $H + C_2H_4 \rightarrow C_2H_5$

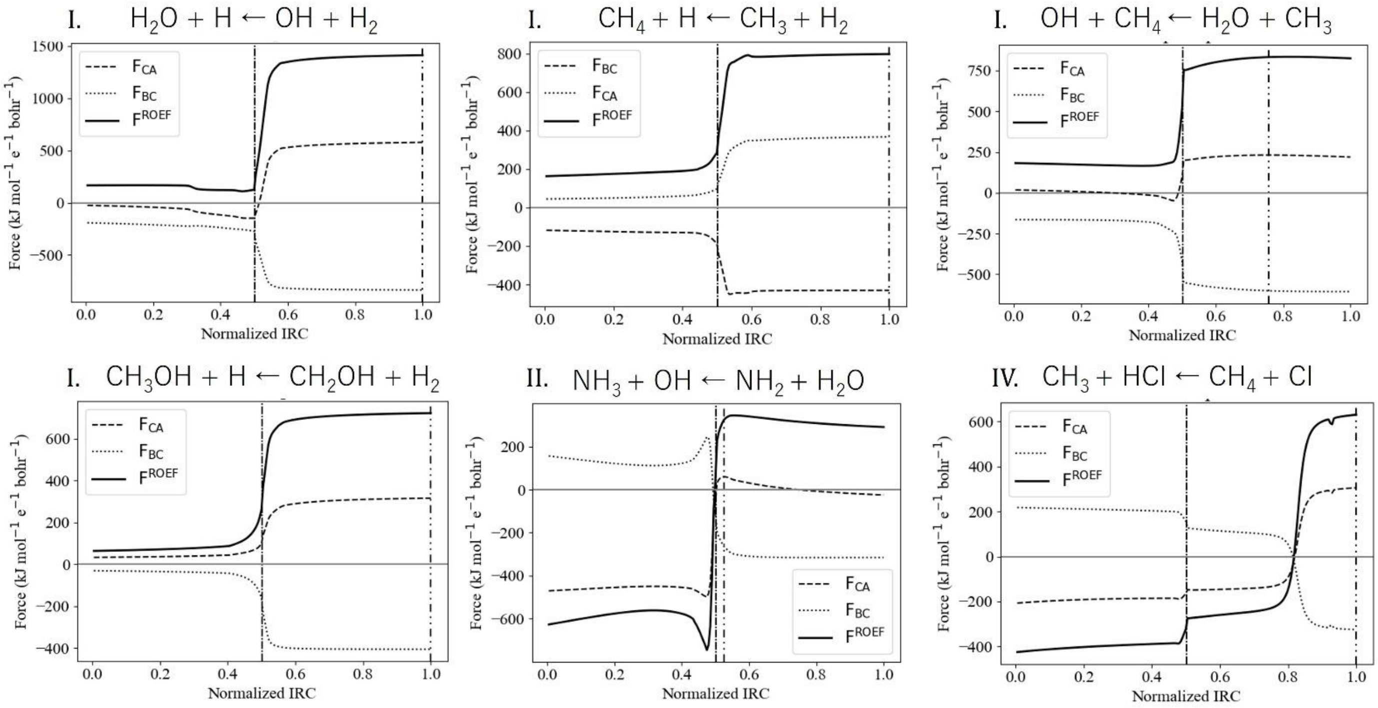


I. $CH_3 + C_2H_4 \rightarrow C_3H_7$



IV. $HCN \rightarrow HNC$

Figure S2. Variations in reactive orbital-based electrostatic force (ROEF) vectors along the B-C and C-A bond directions, represented by F_{BC} (red curves) and F_{CA} (blue curves), against the normalized intrinsic reaction coordinates (IRCs). These ROEF vector variations correspond to characteristic atom transfer reactions and are categorized into four types: I. Continuous forward ROEFs throughout the reaction, II. Sudden reaction-forward ROEFs just before the transition states (TSs), III. Forward ROEFs persisting until reaching the TSs followed by backward ROEFs, and IV. Backward ROEFs after the TSs, for backward processes. The variations are shown only for representative reactions of these types. ROEFs are derived from occupied reactive orbitals, as described in Eq. (8). The definitions for the vectors of F_{BC} and F_{CA} are detailed in Fig. 1(b). Green dotted lines mark the TS locations, while orange dotted lines indicate points where the combined ROEF values directed towards the reaction, F_{CA} - F_{BC}, reach their maximum. In parentheses attaching reaction formulae, the spin states of the reactive molecular orbitals that give larger maximum ROEF values are indicated.



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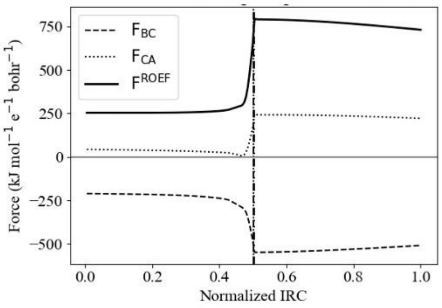

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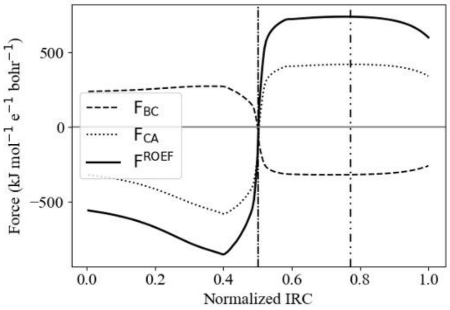

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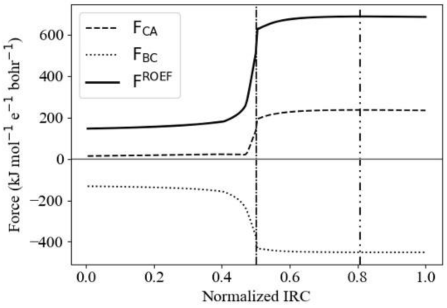

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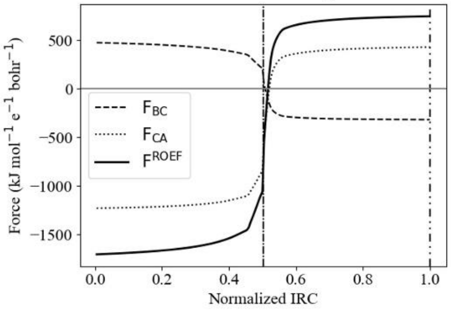

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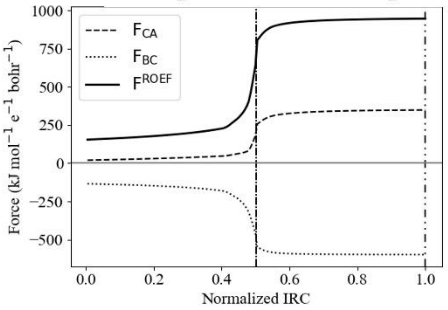

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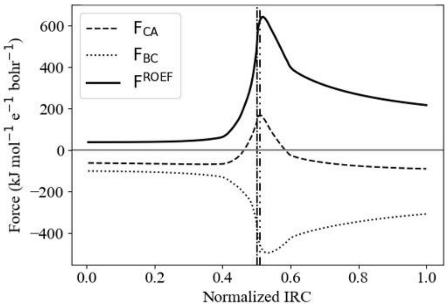

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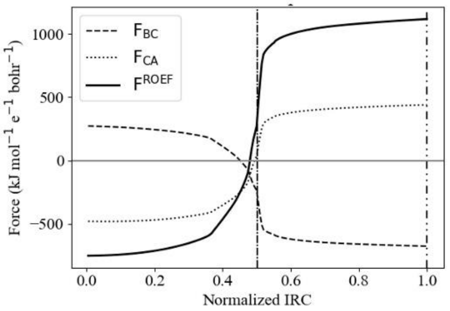

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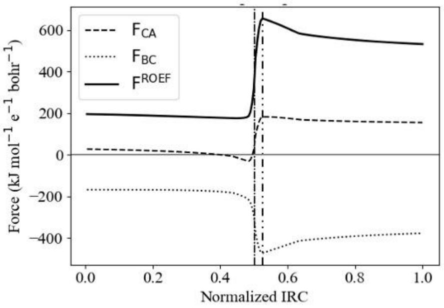

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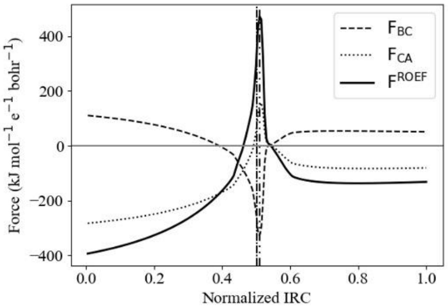

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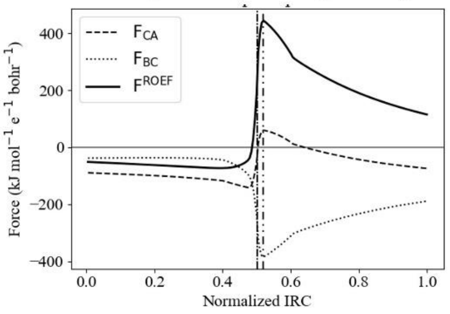

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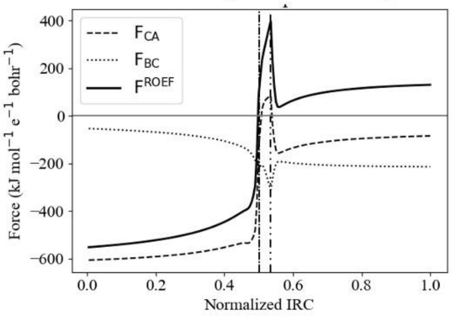

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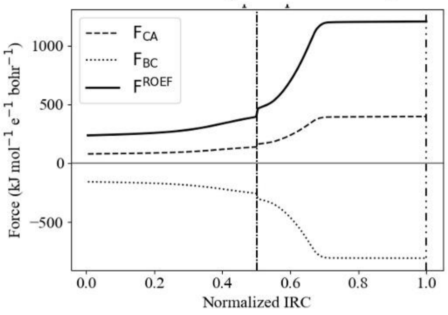

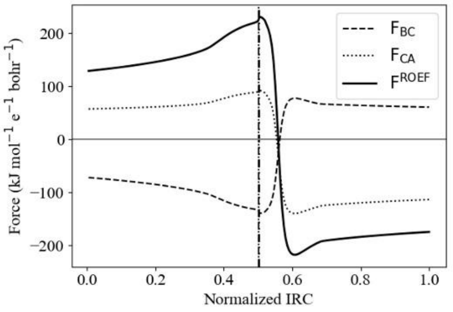

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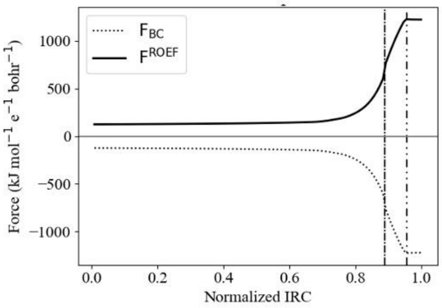

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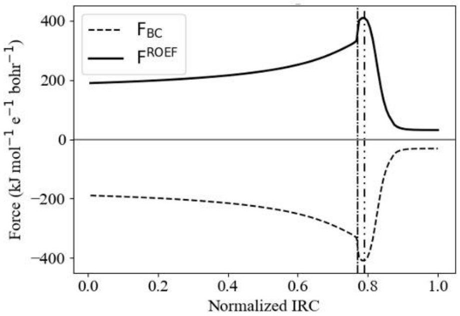

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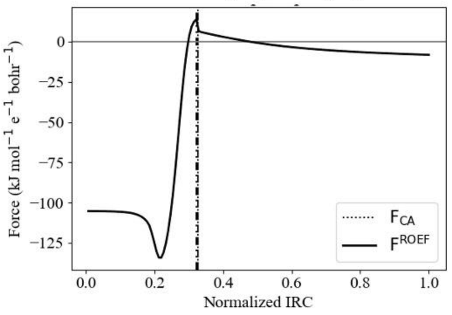

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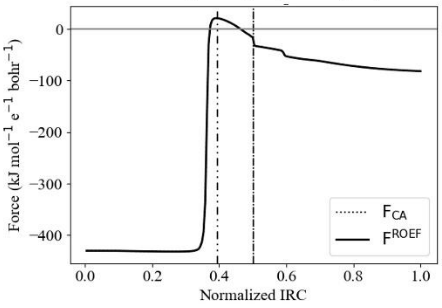

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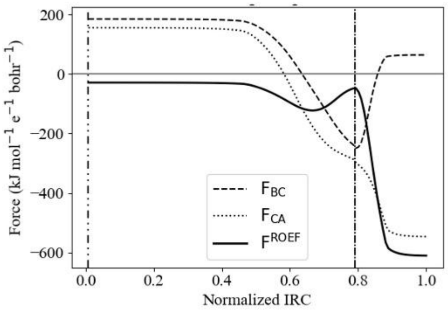

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