In What Ways Do We Characterize Reactions?

$$2\,H_2 \ + \ O_2 \ \longrightarrow \ 2\,H_2O$$

What can we know about this reaction?

In What Ways Do We Characterize Reactions?
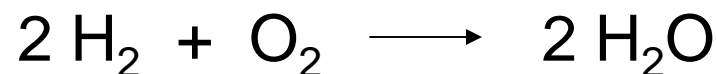
$$2 H_2 + O_2 \longrightarrow 2 H_2O$$

- Identify reactants and products.

- Determine/predict reaction enthalpy (ΔH) or energy (ΔG).

e.g., heats of formation
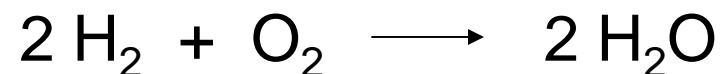
$-2(\Delta H_{f,H_2})$	0
$-(\Delta H_{f,O_2})$	0
$2(\Delta H_{f,H_2O})$	2(-68.3 kcal/mol)

ΔH_{rxn} = $\quad$ -137 kcal/mol

or bond dissociation energies

$2(BDE_{H-H})$	2(104 kcal/mol)
$BDE_{O=O}$	119 kcal/mol
$-4(BDE_{O-H})$	4(111 kcal/mol)

ΔH_{rxn} $\approx$ $\quad$ -117 kcal/mol

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Reaction Thermodynamics

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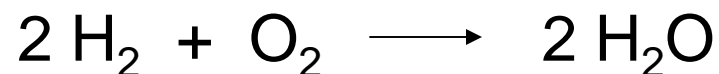
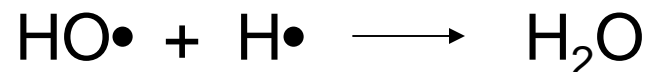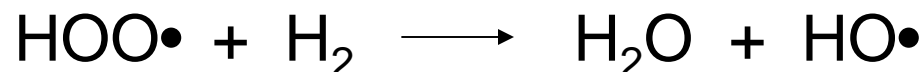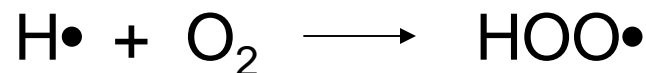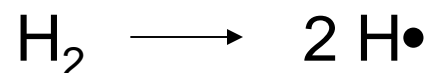$$2\,H_2 + O_2 \longrightarrow 2\,H_2O$$

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Reaction Thermodynamics

- Propose reaction intermediates, transition states.

In What Ways Do We Characterize Reactions?

$$2\ H_2\ +\ O_2\ \longrightarrow\ 2\ H_2O$$

$$H_2\ \longrightarrow\ 2\ H\bullet$$

$$H\bullet\ +\ O_2\ \longrightarrow\ HOO\bullet$$

$$HOO\bullet\ +\ H_2\ \longrightarrow\ H_2O\ +\ HO\bullet$$

$$HO\bullet\ +\ H\bullet\ \longrightarrow\ H_2O$$

Can propose lots of intermediates, multistep mechanisms for reactions. How do we know which of these are correct?

In What Ways Do We Characterize Reactions?
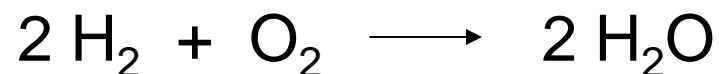
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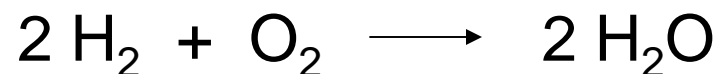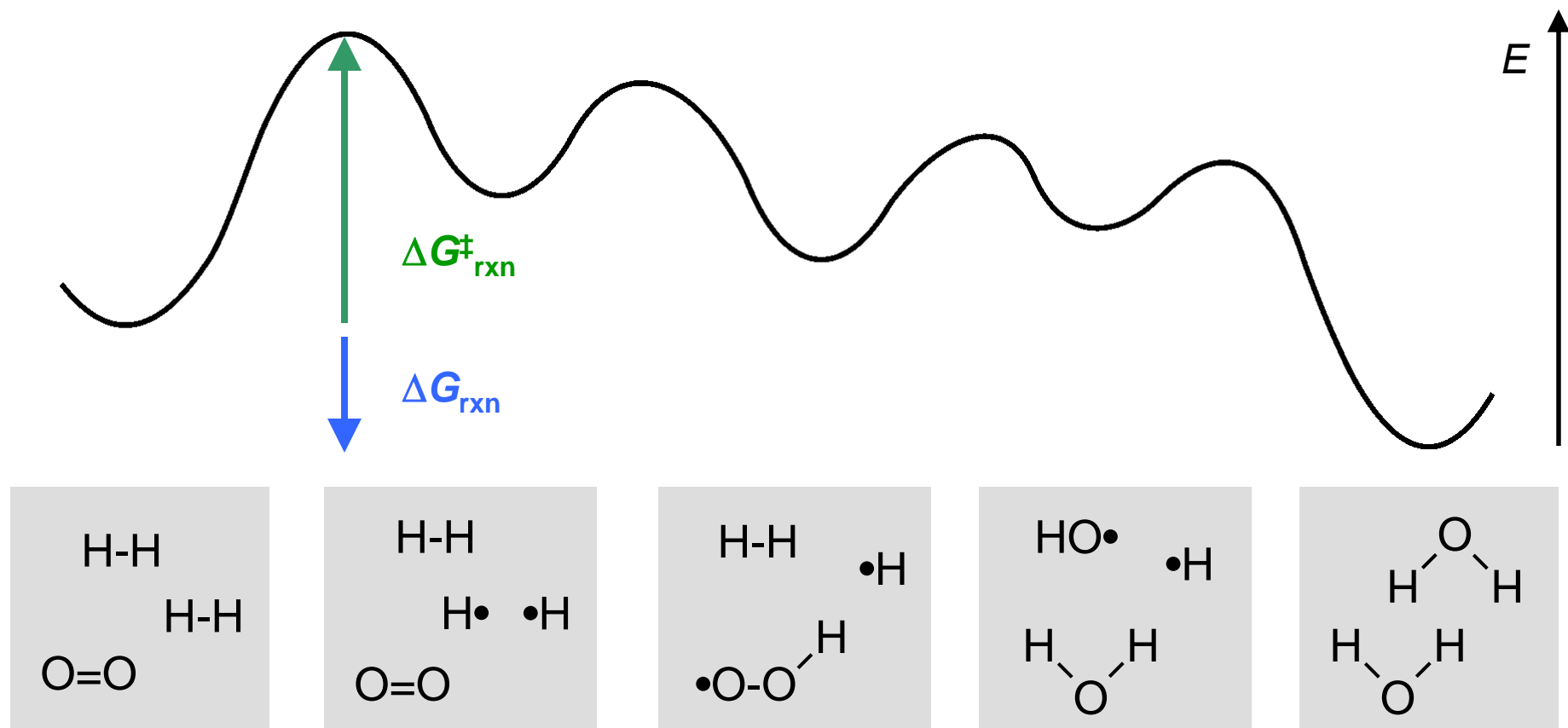
Reaction Thermodynamics

- Propose reaction intermediates, transition states.

- Determine/predict reaction rates.

In What Ways Do We Characterize Reactions?

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O$$

E

$\Delta G^{\ddagger}_{rxn}$

ΔG_{rxn}

H-H
 	
H-H
O=O
	H-H
	
	H• •H
	O=O
		H-H
		  •H
		
		H
		•O-O
			HO•
			  •H
			
			H H
			O
				O
				H H
				
				H H
				O

(Energies not drawn to scale)

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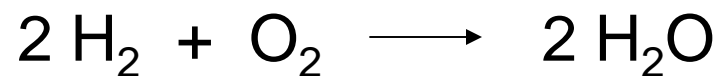
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Reaction Thermodynamics

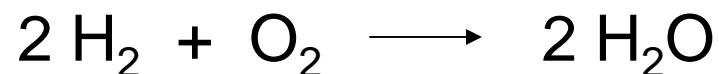- Propose reaction intermediates, transition states.
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Reaction Kinetics