

pullback adjoint bond energy

$$E = K (r - R)^2 \quad \begin{array}{l} \mathbf{r}_1 = (x_1, y_1, z_1) \\ \mathbf{r}_2 = (x_2, y_2, z_2) \end{array}$$
$$r = \|\mathbf{r}_1 - \mathbf{r}_2\|$$

$$\bar{K} = \frac{\partial E}{\partial K} \bar{E} = (r - R)^2 \bar{E}$$

$$\bar{R} = \frac{\partial E}{\partial R} \bar{E} = -2K(r - R) \bar{E}$$

$$\begin{aligned} \bar{x}_1 &= \frac{\partial E}{\partial x_1} \bar{E} = 2K(r - R) \frac{\partial r}{\partial x_1} \bar{E} \\ &= 2K(r - R) \frac{\partial}{\partial x_1} [(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2]^{\frac{1}{2}} \\ &= 2K(r - R) \times \frac{1}{2r} \times 2(x_1 - x_2) \times \bar{E} \\ &= \frac{2K(r - R)}{r} \times (x_1 - x_2) \bar{E} \end{aligned}$$

$$\bar{y}_1 = \frac{2K(r - R)}{r} \times (y_1 - y_2) \bar{E}$$

$$\bar{z}_1 = \frac{2K(r - R)}{r} \times (z_1 - z_2) \bar{E}$$