

**Supporting information for:**

**Simultaneous Visualization of Covalent and  
Non-Covalent Interactions Using Regions of Density  
Overlap**

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# 1 Single-Exponential Decay Detector (SEDD) (Eq. 1)

$$SEDD(\mathbf{r}) = \ln \left[ 1 + \left( \frac{\nabla \left( \frac{\nabla \rho(\mathbf{r})}{\rho(\mathbf{r})} \right)^2}{\rho(\mathbf{r})} \right)^2 \right] = \ln [1 + \xi(\mathbf{r})]$$

$$\xi(\mathbf{r}) = \left( \frac{\nabla \left( \frac{\nabla \rho(\mathbf{r})}{\rho(\mathbf{r})} \right)^2}{\rho(\mathbf{r})} \right)^2 = \frac{1}{(\rho(\mathbf{r}))^2} \left\{ \left[ \nabla \left( \frac{\nabla \rho(\mathbf{r}) \cdot \nabla \rho(\mathbf{r})}{(\rho(\mathbf{r}))^2} \right) \right] \cdot \left[ \nabla \left( \frac{\nabla \rho(\mathbf{r}) \cdot \nabla \rho(\mathbf{r})}{(\rho(\mathbf{r}))^2} \right) \right] \right\}$$

$$\xi(\mathbf{r}) = \frac{4}{(\rho(\mathbf{r}))^8} \left\{ \begin{aligned} & \left[ \rho(\mathbf{r}) \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \frac{\partial^2 \rho(\mathbf{r})}{\partial x^2} + \frac{\partial \rho(\mathbf{r})}{\partial y} \frac{\partial^2 \rho(\mathbf{r})}{\partial x \partial y} + \frac{\partial \rho(\mathbf{r})}{\partial z} \frac{\partial^2 \rho(\mathbf{r})}{\partial x \partial z} \right) - \right. \\ & \left. \frac{\partial \rho(\mathbf{r})}{\partial x} \left( \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial y} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial z} \right)^2 \right) \right]^2 + \\ & \left[ \rho(\mathbf{r}) \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \frac{\partial^2 \rho(\mathbf{r})}{\partial x \partial y} + \frac{\partial \rho(\mathbf{r})}{\partial y} \frac{\partial^2 \rho(\mathbf{r})}{\partial y^2} + \frac{\partial \rho(\mathbf{r})}{\partial z} \frac{\partial^2 \rho(\mathbf{r})}{\partial y \partial z} \right) - \right. \\ & \left. \frac{\partial \rho(\mathbf{r})}{\partial y} \left( \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial y} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial z} \right)^2 \right) \right]^2 + \\ & \left[ \rho(\mathbf{r}) \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \frac{\partial^2 \rho(\mathbf{r})}{\partial x \partial z} + \frac{\partial \rho(\mathbf{r})}{\partial y} \frac{\partial^2 \rho(\mathbf{r})}{\partial y \partial z} + \frac{\partial \rho(\mathbf{r})}{\partial z} \frac{\partial^2 \rho(\mathbf{r})}{\partial z^2} \right) - \right. \\ & \left. \frac{\partial \rho(\mathbf{r})}{\partial z} \left( \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial y} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial z} \right)^2 \right) \right]^2 + \end{aligned} \right\}$$

## 2 Density Overlap Regions Indicator (DORI) (Eqs. 2 and 3)

$$DORI(\mathbf{r}) = \frac{\theta(\mathbf{r})}{1 + \theta(\mathbf{r})}$$

$$\begin{aligned} \theta(\mathbf{r}) &= \frac{\left( \nabla \left( \frac{\nabla \rho(\mathbf{r})}{\rho(\mathbf{r})} \right)^2 \right)^2}{\left( \frac{\nabla \rho(\mathbf{r})}{\rho(\mathbf{r})} \right)^6} \\ &= \left\{ \left[ \nabla \left( \frac{\nabla \rho(\mathbf{r}) \cdot \nabla \rho(\mathbf{r})}{(\rho(\mathbf{r}))^2} \right) \right] \cdot \left[ \nabla \left( \frac{\nabla \rho(\mathbf{r}) \cdot \nabla \rho(\mathbf{r})}{(\rho(\mathbf{r}))^2} \right) \right] \right\} \left\{ \left( \frac{\nabla \rho(\mathbf{r}) \cdot \nabla \rho(\mathbf{r})}{(\rho(\mathbf{r}))^2} \right)^3 \right\}^{-1} \end{aligned}$$

$$\begin{aligned} \xi(\mathbf{r}) &= \frac{4}{\left( \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial y} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial z} \right)^2 \right)^3} \left\{ \right. \\ &\quad \left[ \rho(\mathbf{r}) \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \frac{\partial^2 \rho(\mathbf{r})}{\partial x^2} + \frac{\partial \rho(\mathbf{r})}{\partial y} \frac{\partial^2 \rho(\mathbf{r})}{\partial x \partial y} + \frac{\partial \rho(\mathbf{r})}{\partial z} \frac{\partial^2 \rho(\mathbf{r})}{\partial x \partial z} \right) - \right. \\ &\quad \left. \left. \frac{\partial \rho(\mathbf{r})}{\partial x} \left( \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial y} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial z} \right)^2 \right) \right]^2 + \\ &\quad \left[ \rho(\mathbf{r}) \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \frac{\partial^2 \rho(\mathbf{r})}{\partial x \partial y} + \frac{\partial \rho(\mathbf{r})}{\partial y} \frac{\partial^2 \rho(\mathbf{r})}{\partial y^2} + \frac{\partial \rho(\mathbf{r})}{\partial z} \frac{\partial^2 \rho(\mathbf{r})}{\partial y \partial z} \right) - \right. \\ &\quad \left. \left. \frac{\partial \rho(\mathbf{r})}{\partial y} \left( \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial y} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial z} \right)^2 \right) \right]^2 + \\ &\quad \left[ \rho(\mathbf{r}) \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \frac{\partial^2 \rho(\mathbf{r})}{\partial x \partial z} + \frac{\partial \rho(\mathbf{r})}{\partial y} \frac{\partial^2 \rho(\mathbf{r})}{\partial y \partial z} + \frac{\partial \rho(\mathbf{r})}{\partial z} \frac{\partial^2 \rho(\mathbf{r})}{\partial z^2} \right) - \right. \\ &\quad \left. \left. \frac{\partial \rho(\mathbf{r})}{\partial z} \left( \left( \frac{\partial \rho(\mathbf{r})}{\partial x} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial y} \right)^2 + \left( \frac{\partial \rho(\mathbf{r})}{\partial z} \right)^2 \right) \right]^2 + \\ &\quad \left. \right\} \end{aligned}$$