

# Supporting Information

## **Influence of $\beta$ -Cyclodextrin Methylation on Host-Guest Complex Stability: A Theoretical Study of Intra- and Intermolecular Interactions as well as Host Dimer Formation**

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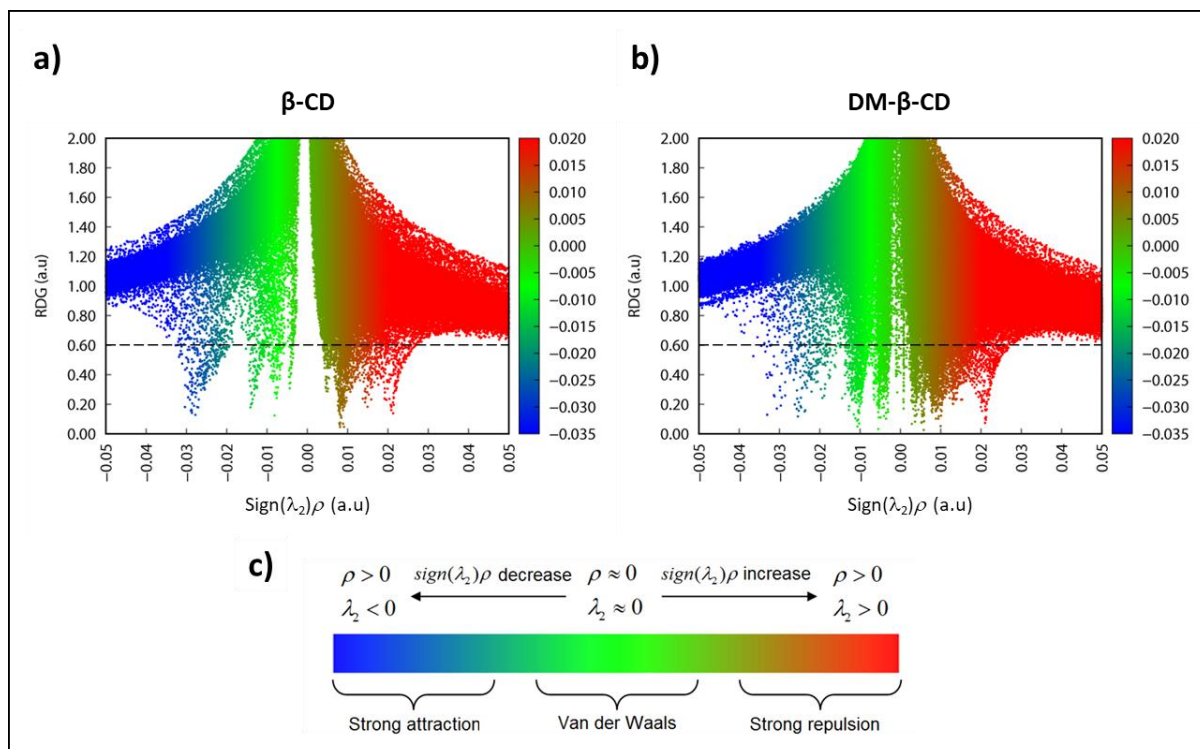
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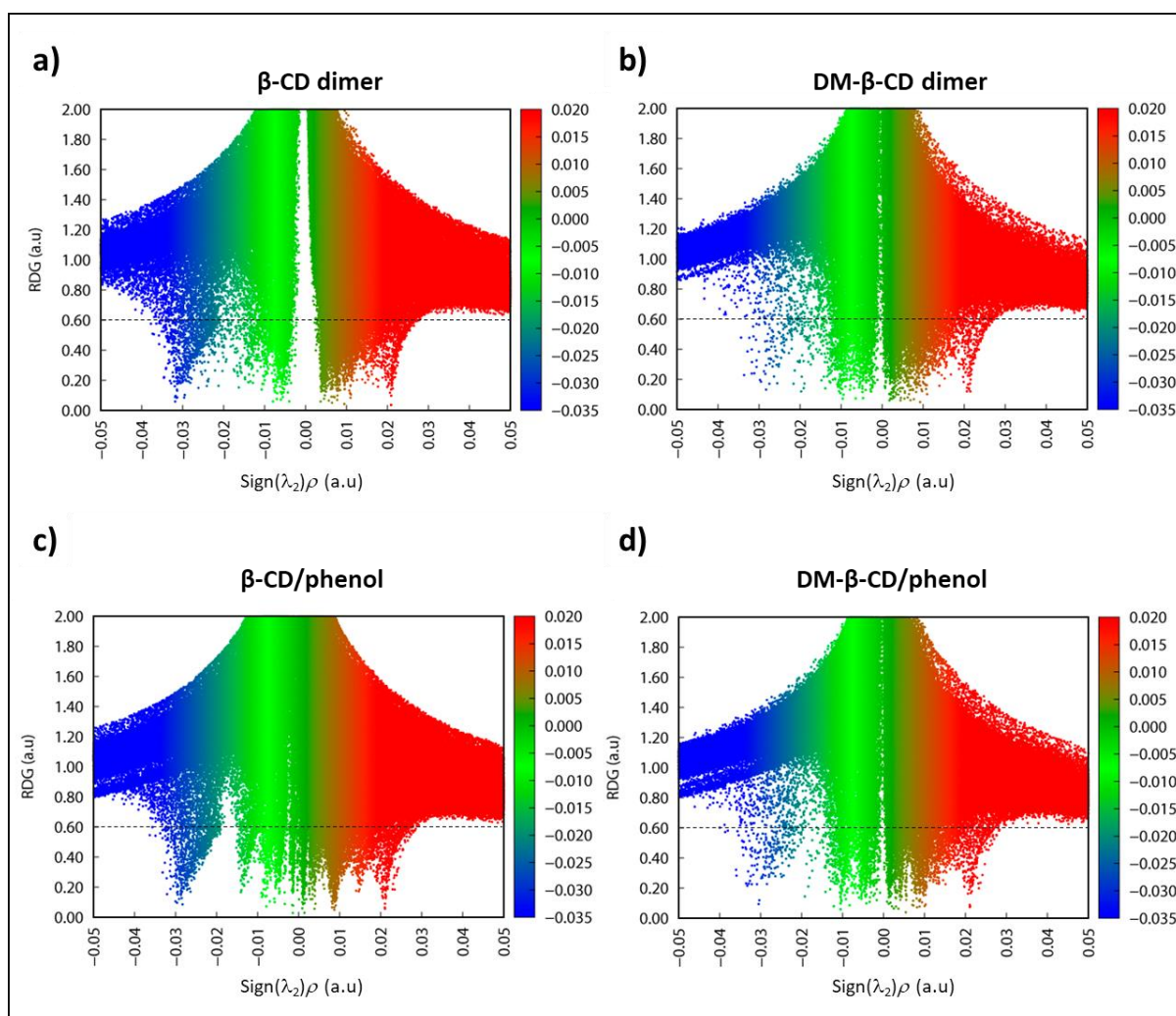
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**Figure S2.** Color-filled scatter plots of the reduced density gradient versus the sign of the second Hessian eigenvalue, multiplied by the electron density of a) the  **$\beta$ -CD dimer**, b) the **DM- $\beta$ -CD dimer**, c) the  **$\beta$ -CD/phenol** complex and d) the **DM- $\beta$ -CD/phenol** complex. The data was obtained by evaluating the B97-3c density. To cover the entire system, the grid configuration used was around 1728000 points in total. .... 4



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**Figure S2.** Color-filled scatter plots of the reduced density gradient versus the sign of the second Hessian eigenvalue, multiplied by the electron density of a) the  **$\beta$ -CD dimer**, b) the **DM- $\beta$ -CD dimer**, c) the  **$\beta$ -CD/phenol** complex and d) the **DM- $\beta$ -CD/phenol** complex. The data was obtained by evaluating the B97-3c density. To cover the entire system, the grid configuration used was around 1728000 points in total.