

ab-initio based **bulk** charge density $n(\mathbf{r})$



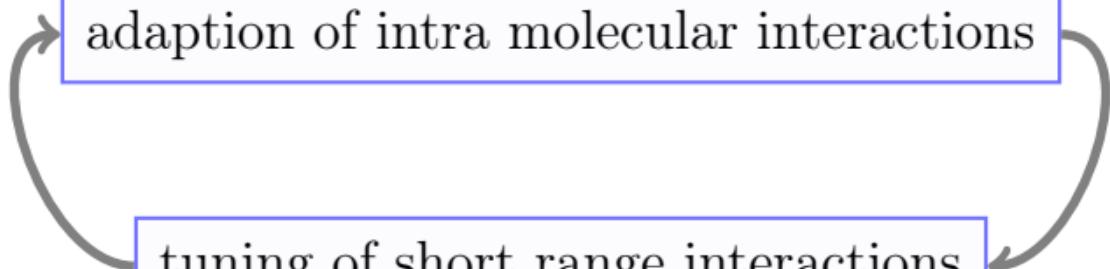
calculation of model charge density $\tilde{n}(\mathbf{r})$



partial charges



adaption of intra molecular interactions



tuning of short range interactions



force field validation