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### **Bayesian Error Estimation Functionals**

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The challenge of approximating the exchange-correlation functional in Density Functional Theory (DFT) has led to the development of numerous different approximations of varying accuracy on different calculated properties. There is therefore a need for reliable estimation of prediction errors within the different approximation schemes to DFT. The Bayesian Error Estimation Functionals (BEEF) have been developed with this in mind. The functionals are constructed by fitting to experimental and high-quality computational databases for molecules and solids including chemisorption and van der Waals systems. This leads to reasonably accurate general-purpose functionals with particular focus on surface science. The fitting procedure involves considerations on how to combine different types of data, and applies Tikhonov regularization and bootstrap cross validation. The methodology has been applied to construct GGA and metaGGA functionals with and without inclusion of long-ranged van der Waals contributions. The error estimation is made possible by the generation of not only a single functional but through the construction of a probability distribution of functionals represented by a functional ensemble. The use of the functional ensemble is illustrated on compound heat of formation and by investigations of the reliability of calculated catalytic ammonia synthesis rates.