INVESTIGATING POPULAR WATER MODELS

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A detailed analysis of the various terms - electrostatics, polarization and repulsion/dispersion present in several popular water models will be presented. It is shown, that even the most successful models have deficiencies. With the aid of MP2 calculations we have reparameterized the TTM2-R and AMOEBA water models. These reparameterized models are tested on several water clusters and for bulk water.