1. What is the purpose of this work? How the system of protein and water needs to be constructed and modeled.

建立一个合理的水分子间势能模型（包含平均多体相互作用），进行水合蛋白的动力学模拟

文本, 信件

描述已自动生成

1. What is the problem to build an ab initio potential? What is effective pair-additive potential?

pair-additive potential：总势能是粒子对势能之和

effective pair-additive potential：通过

文本, 信件

描述已自动生成

文本

低可信度描述已自动生成

1. In this work what degrees of freedom are considered for building a water potential function? Why does the author describe the molecule as rigid?

水分子结构数据是相对固定的，因而可以采用刚性模型（忽略振动和伸缩）

1. In the frame of this model, describe the interactions between protein and water molecules.
2. How is liquid water represented in computer simulations?
3. How do the authors describe the hydrogen bonds?

Omit

1. Define the radial distribution function. How is it related to the intermolecular parameters?
2. What may be missing in the pairwise interaction? How is this problem solved?
3. How many adjustable parameters in this model? How are these parameters determined?