# Article information:

Investigation on the interfacial behavior of polyorganic inhibitors on a metal surface by DFT study and MD simulation - ScienceDirect  
<https://www.sciencedirect.com/science/article/abs/pii/S0169433220333286?via%3Dihub=>

# Article summary:

1. Corrosion inhibitors can be added to industrial processes to prevent metal equipment from corroding, and computational chemistry methods such as DFT and MD simulations are used to investigate the interfacial behavior of these inhibitors on metal surfaces.

2. The effect of the degree of polymerization (DP) on the adsorption behavior of polyorganic inhibitors (PEG and PAM) on metallic iron surfaces was studied using DFT and MD simulation.

3. Both PEG and PAM can be adsorbed on metallic iron surfaces via a preliminary mechanism in which the HOMO orbital combines with the d orbitals of the metal surface, but the DP affects their adsorption behavior differently.

# Article rating:

Appears moderately imbalanced: The article provides some useful information, but is missing several important points or pieces of evidence that would be required to present the discussed topics in a balanced and reliable way. You are encouraged to seek a more balanced perspective on the presented issues by exploring the provided research topics and looking at different information sources.

# Article analysis:

该文章主要介绍了利用DFT和MD模拟研究有机缓蚀剂在金属表面的界面行为。文章提到，传统的实验方法存在盲目性、工作量大、时间长等局限性，因此计算化学方法成为了研究有机缓蚀剂与金属表面相互作用的重要手段。作者通过对PEG和PAM两种聚合物的不同聚合度进行模拟研究，探讨了聚合度对有机缓蚀剂在金属表面吸附行为的影响。

然而，该文章存在以下问题：

1. 缺乏实验验证：虽然作者提到传统实验方法存在局限性，但是没有提供任何实验数据来验证模拟结果的准确性和可靠性。

2. 偏重于理论分析：文章过于强调计算化学方法在研究有机缓蚀剂与金属表面相互作用方面的优势，但忽略了实际应用中其他因素的影响。例如，在现实环境中，温度、压力、流速等因素都会影响有机缓蚀剂在金属表面上的吸附行为。

3. 缺乏对环境风险和健康安全的考虑：文章提到研究环保型缓蚀剂的重要性，但没有对传统缓蚀剂可能带来的环境风险和健康安全问题进行讨论。

4. 缺乏对不同金属材料的研究：文章只针对铁材料进行了模拟研究，而忽略了其他金属材料在实际应用中的广泛使用。

5. 结论不够明确：文章提出了PEG和PAM两种聚合物在金属表面吸附行为的机制，但是并没有给出具体的结论或建议，无法为实际应用提供指导意义。

综上所述，该文章存在一定程度上的片面性和局限性，在实际应用中需要更多方面的考虑和验证。

# Topics for further research:

* Experimental validation of simulation results
* Consideration of other factors in practical applications
* Assessment of environmental and health risks
* Investigation of different metal materials
* Clearer conclusions and recommendations
* Limitations and biases of computational chemistry methods

# Report location:

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