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Impact of Nitration on Electroporation Dynamics: Insights from Molecular Dynamics Simulations for Biomedical Applications

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Electroporation, the temporary increase in cell membrane permeability caused by electric fields, is a fundamental technique in biomedicine, enabling gene transfer, drug delivery, and cancer treatment.[1,2] However, the effects of nitration—a biochemical modification that introduces nitro groups into phospholipids—on the dynamics of electroporation have not been thoroughly studied. In this research, we use molecular dynamics simulations to investigate how nitration influences pore formation during electroporation. By systematically varying nitration levels and electric field strengths, we examine the intricate interaction between nitration and electroporation kinetics. Our simulations reveal that higher nitration levels significantly accelerate pore formation, with notable reductions in the time required for pore generation observed at increased nitration levels and stronger electric fields (see Figure 1). This finding highlights the role of nitration in modifying the kinetics of electroporation. Furthermore, given its relevance to cold plasma applications, we emphasize the potential implications of these results for cold plasma-mediated cancer therapy and other biomedical treatments.[3] Our study provides a deeper understanding of the mechanisms behind this phenomenon, offering valuable insights for improving electroporation protocols in gene therapy, drug delivery, plasma-based cancer therapy, and related biomedical applications. These findings illuminate the synergistic relationship between nitration, electroporation, and cold plasma, paving the way for future advancements in this critical area of plasma science.

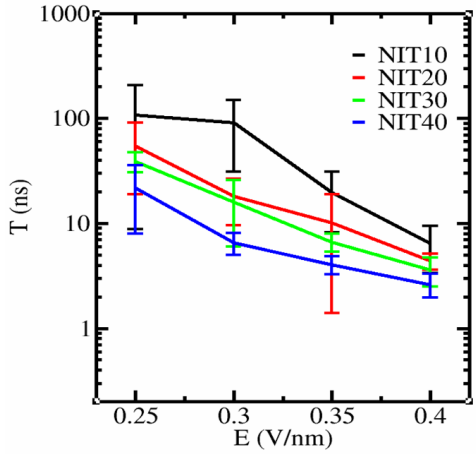

Figure 1. Dependence of the pore formation time on the electric field.

References
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