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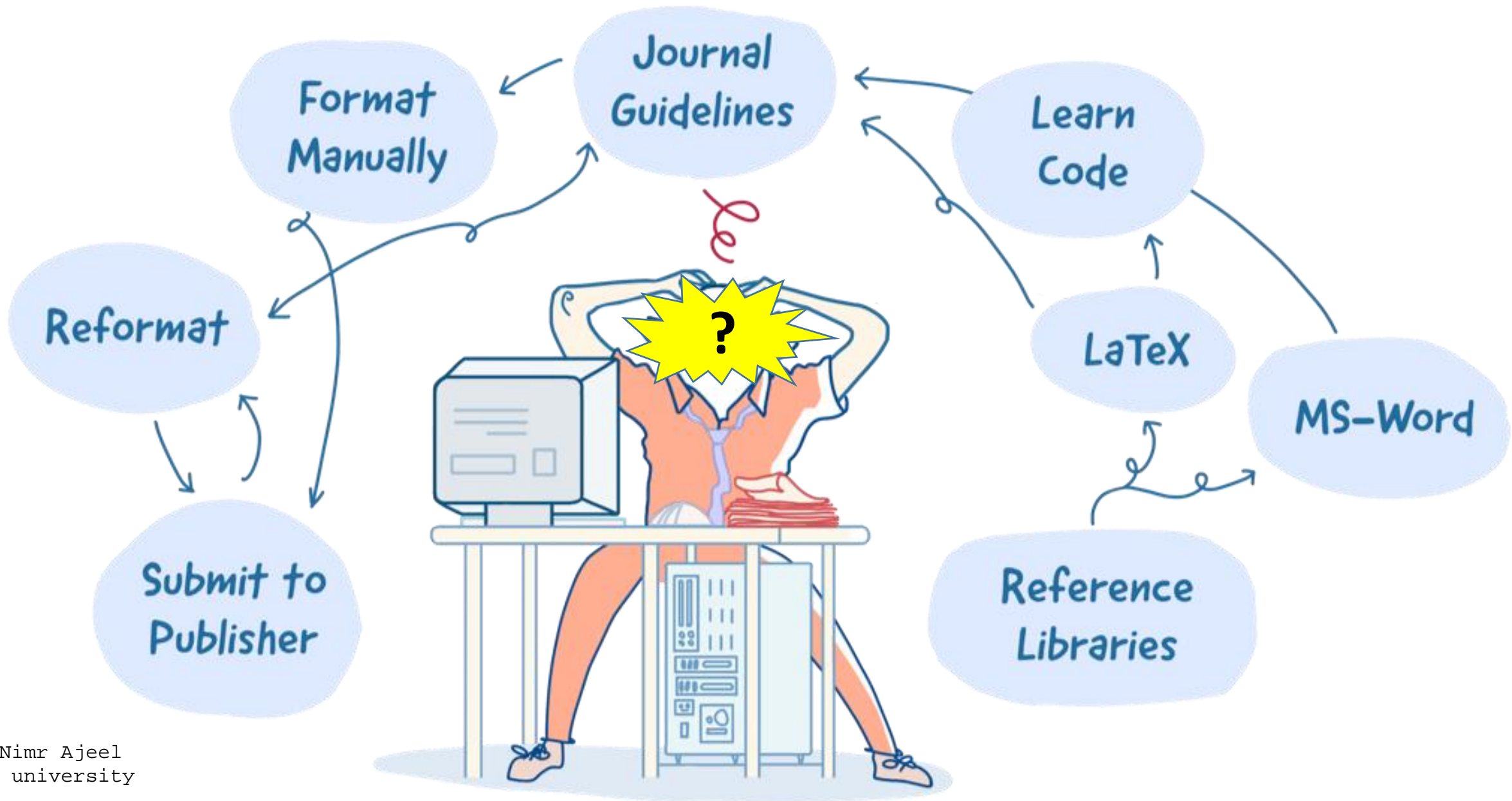


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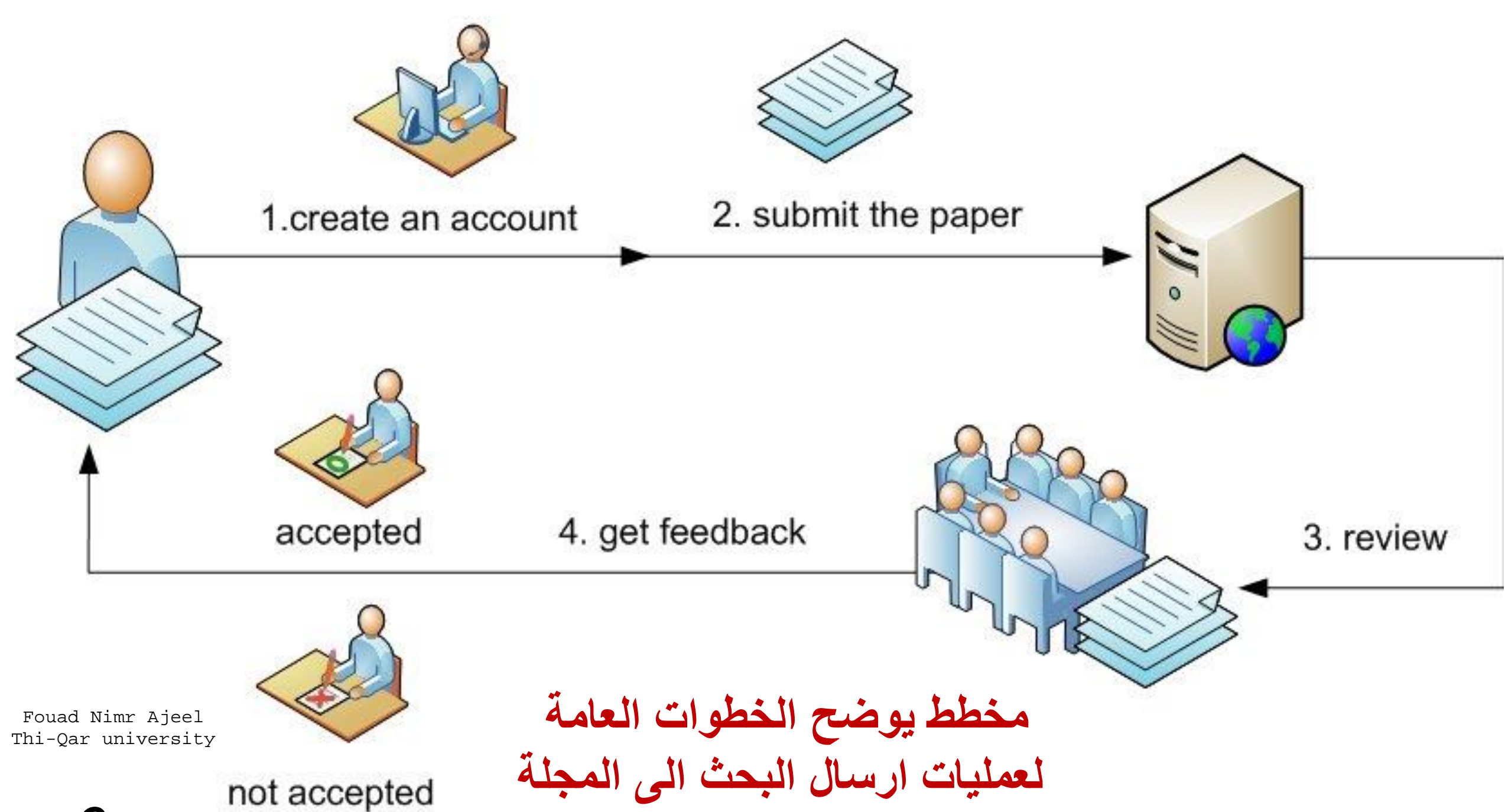




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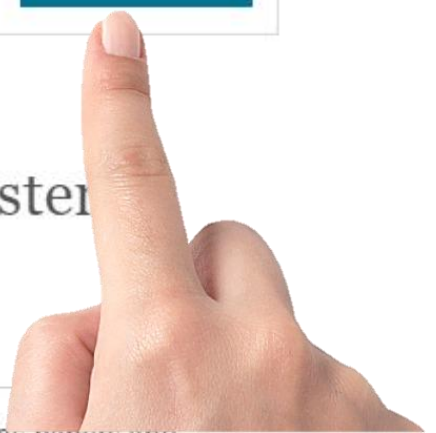
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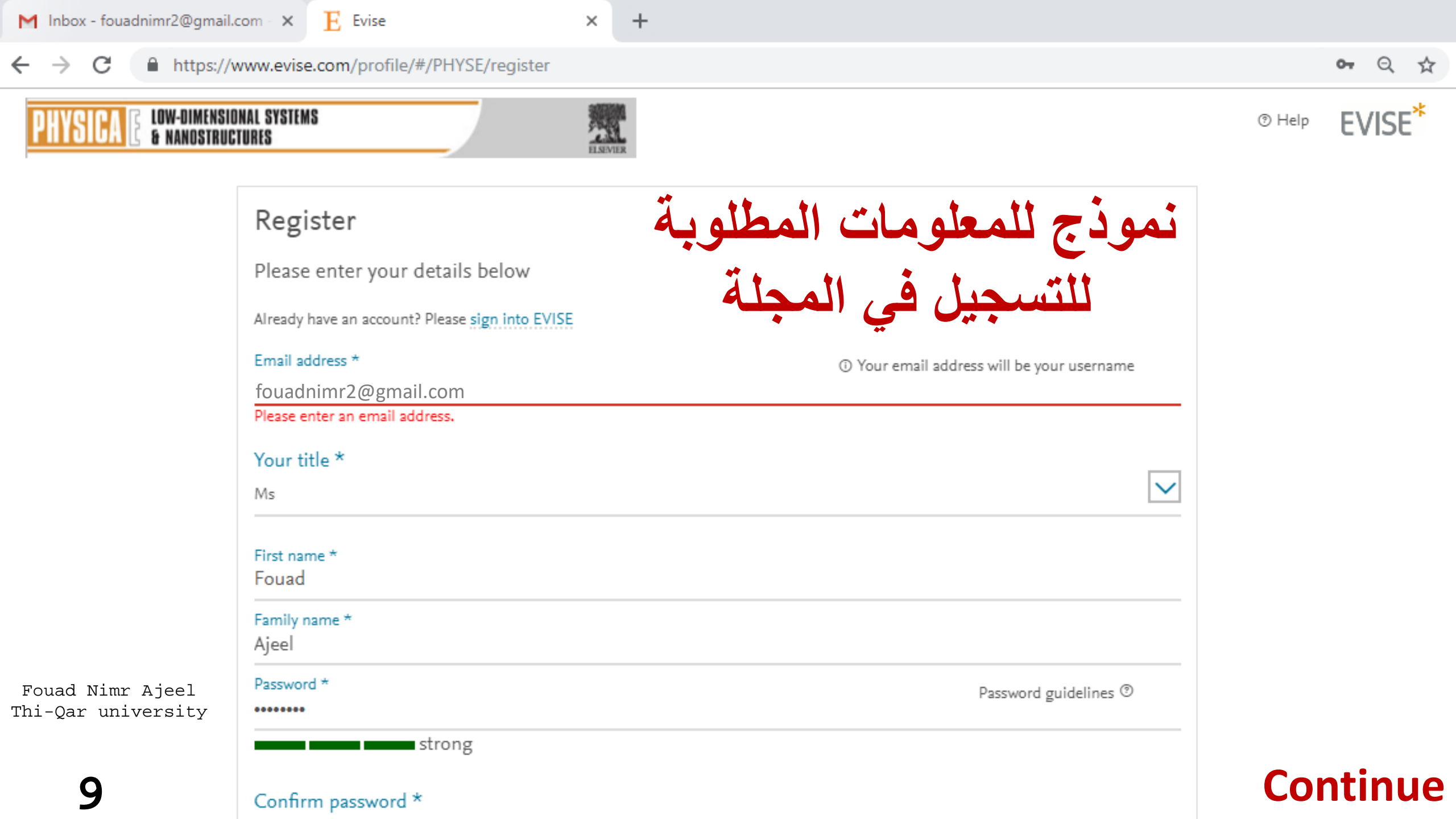
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Energy bandgap engineering is used to produce semiconductor heterostructure systems that perform processes such as the resonant tunneling in nanoelectronics and the solar energy conversion in solar cell applications. However, the performance of such systems degrades as their size is reduced. Graphene-based nanoelectronics has appeared as a candidate to enable high performance down to the single-molecule scale. Here, graphene nanoribbons (GNRs) can have bandgaps that are tunable by

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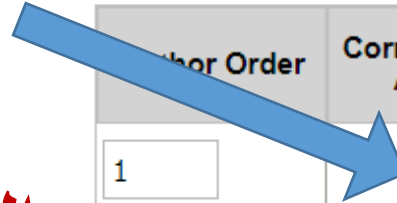
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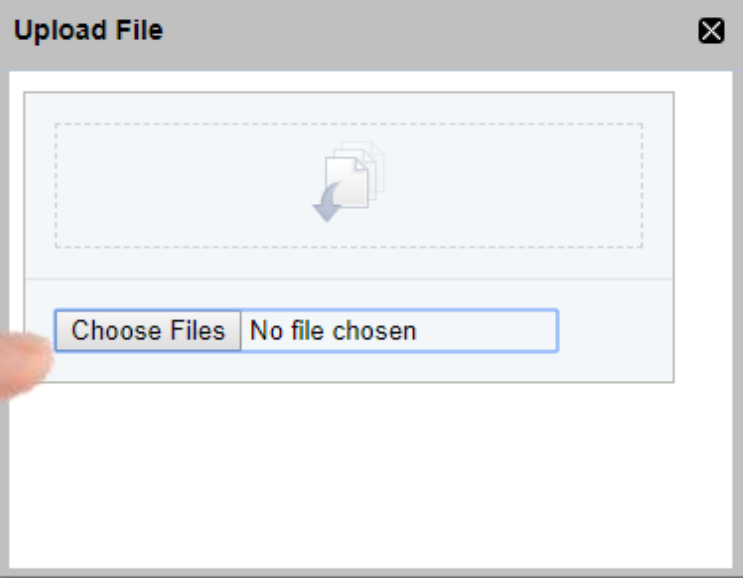
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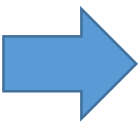
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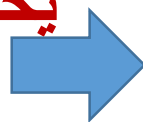
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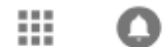
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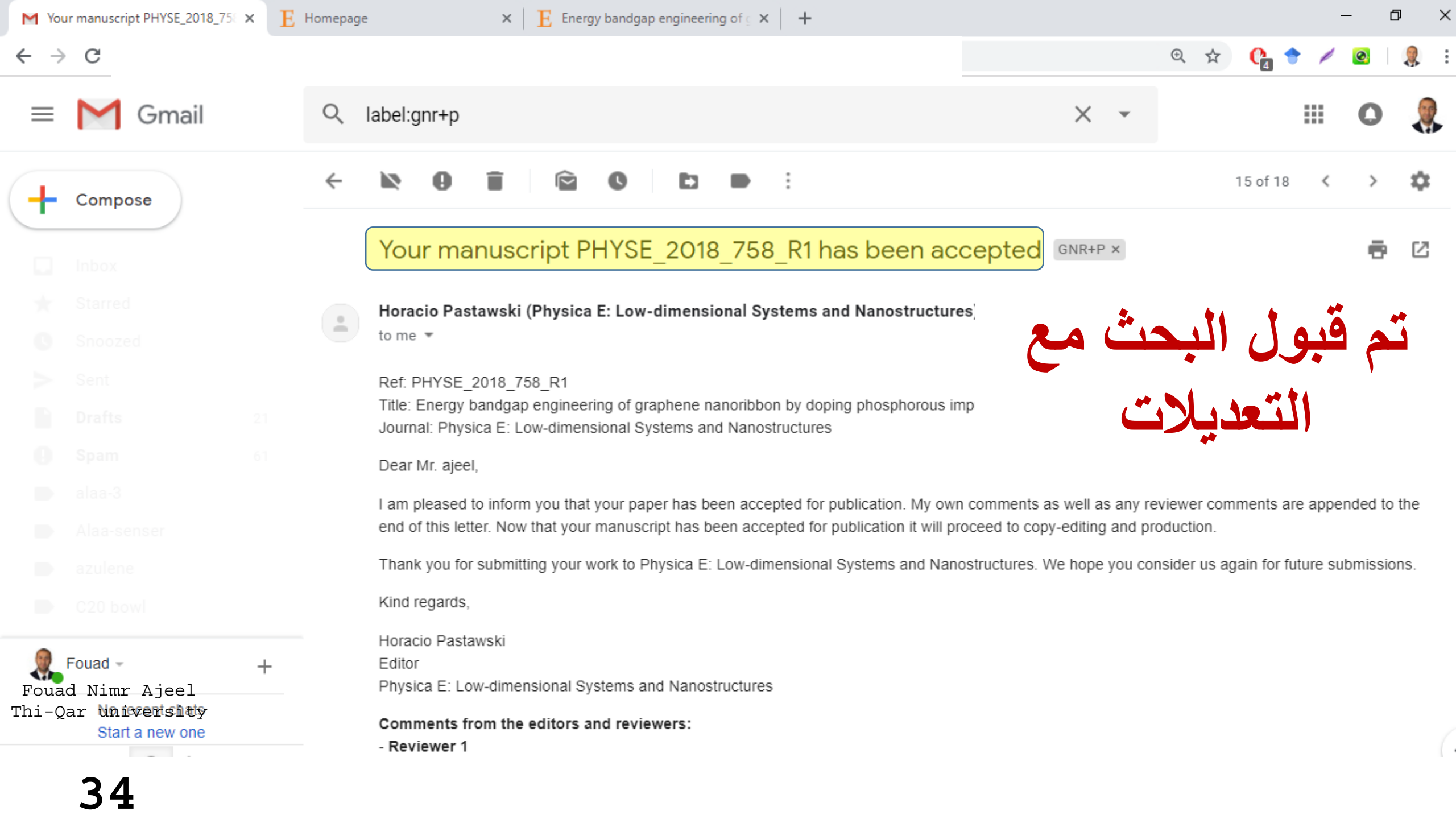
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Abstract

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1. Introduction

2. Computational details

3. Results and discussions

4. Conclusion

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## Energy bandgap engineering of graphene nanoribbon by doping phosphorous impurities to create nano-heterostructures: A DFT study

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<sup>a</sup> Department of Physics, College of Science, University of Thi Qar, Nassiriya 64000, Iraq

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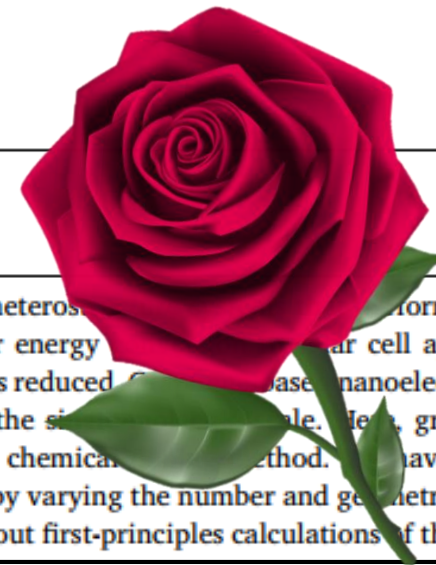
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Energy bandgap engineering is used to produce semiconductor heterostructures to perform processes such as the resonant tunneling in nanoelectronics and the solar energy conversion in solar cell applications. However, the performance of such systems degrades as their size is reduced. Graphene nanoelectronics has appeared as a candidate to enable high performance down to the single molecule level. Here, graphene nanoribbons (GNRs) can have bandgaps that are tunable by using chemical doping method. It has been predicted that bandgap engineering within a GNR may be achieved by varying the number and geometrical pattern of phosphorus (P) impurities in the GNS, so that we have carried out first-principles calculations of the energetic



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