Today I'm going to show you how to calculate the adsorption energy of a molecule adsorbed on a surface. Adsorption energy is a measure of how strongly a molecule binds to a surface, and it can affect many processes such as catalysis, sensors, electronics, and more. Adsorption energy can be calculated using different methods, but in this post I'm going to focus on one of them: the density functional theory (DFT) method.

DFT is a computational method that can solve the quantum mechanical equations for the electrons in a system. DFT can give us accurate information about the electronic and geometric properties of adsorbates (the molecules that are adsorbed) and substrates (the surfaces that they are adsorbed on). To use DFT, we need to create a model of the adsorption system, which usually consists of a slab of the substrate material and one or more adsorbate molecules on top of it. The slab should be thick enough to represent the bulk properties of the substrate, and it should have periodic boundary conditions along the surface plane. The adsorbate molecules should be placed in a reasonable configuration on the surface, depending on the symmetry and chemistry of the system.

Once we have the model, we need to perform DFT calculations for three different cases:

(1) the isolated slab,

(2) the isolated adsorbate molecules, and

(3) the combined slab-adsorbate system.

The DFT calculations will give us the total energies of each case, which we can use to calculate the adsorption energy using this formula:

$$E_{ads} = E_{slab+ads} - E_{iso-slab} - E_{iso-ads}$$

where E_{ads} is the adsorption energy, $E_{slab+ads}$ is the total energy of the combined slab-adsorbate system, $E_{iso-slab}$ is the total energy of the isolated slab, and $E_{iso-ads}$ is the total energy of the isolated adsorbate molecules. The adsorption energy can be positive or negative, depending on whether the adsorption process is endothermic or exothermic. A negative adsorption energy means that the adsorption process releases energy and is favorable, while a positive adsorption energy means that the adsorption process requires energy and is unfavorable. Note: Sometimes researchers adopt the reverse convention where the adsorption energy is calculated as the negative of the previously given formula. In that case, a positive adsorption energy indicates that the adsorption is favorable.

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I hope you enjoyed this blog post and learned something new about adsorption energy calculation using DFT. If you have any questions or comments, feel free to leave them below. Thanks for reading!

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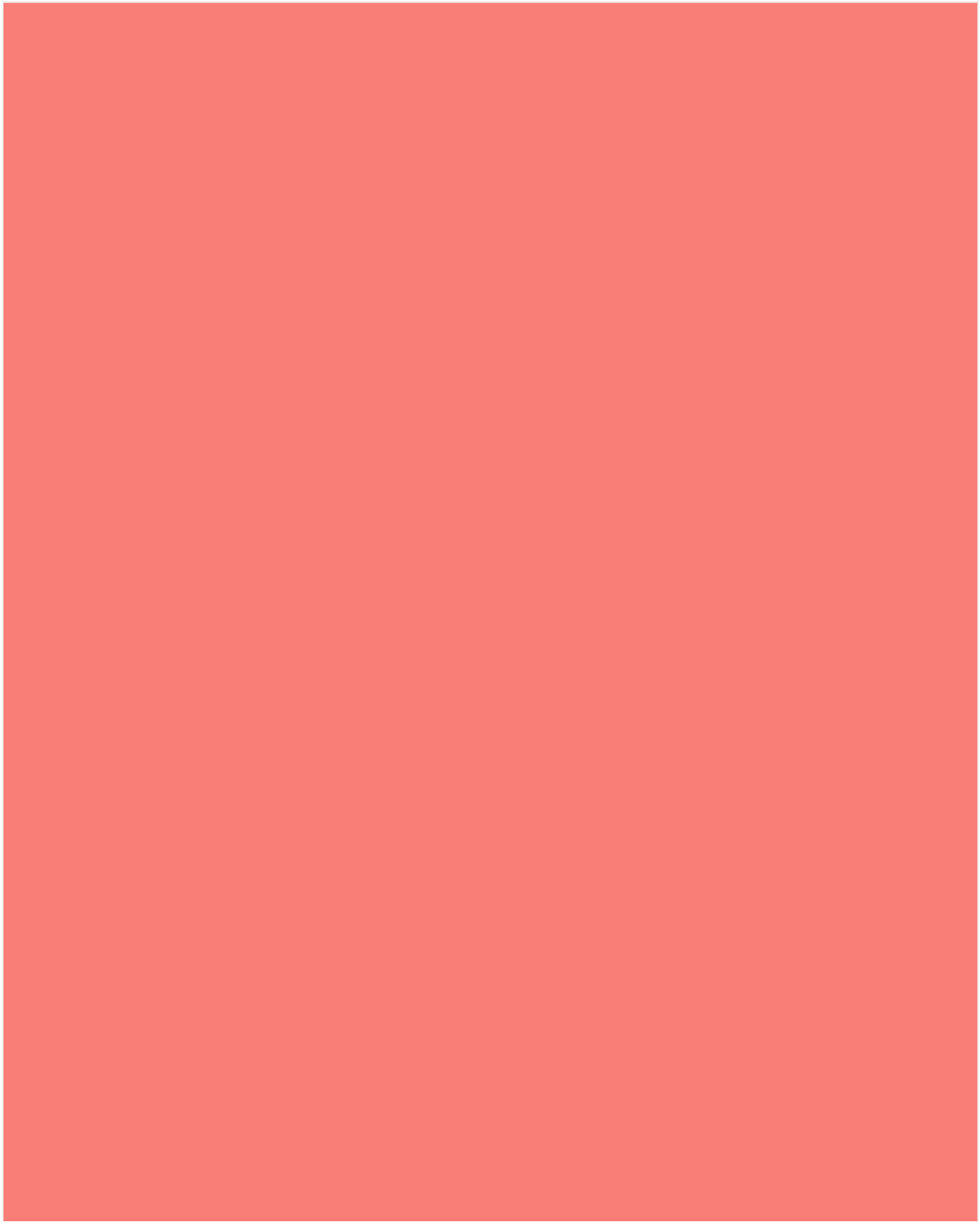

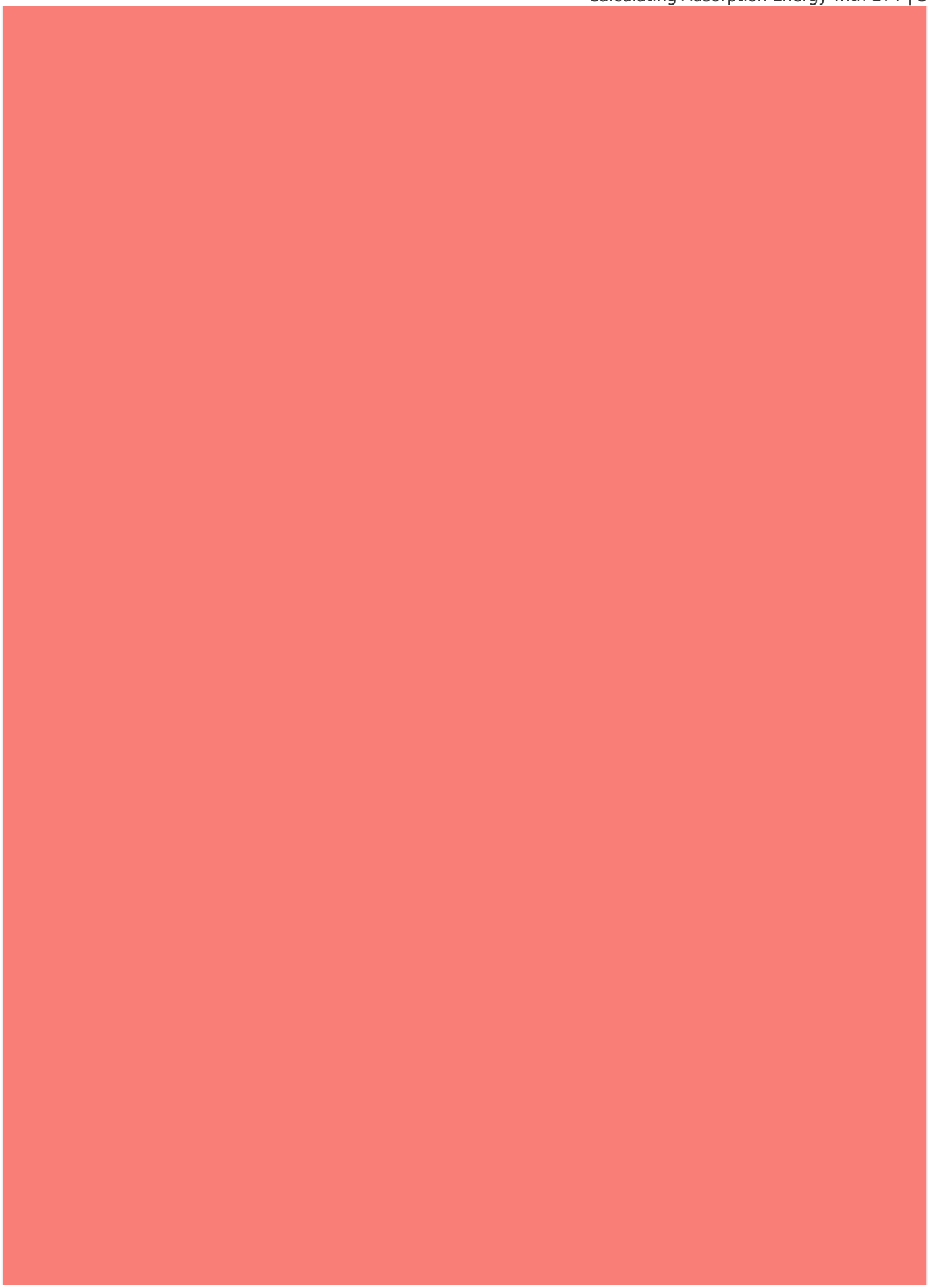

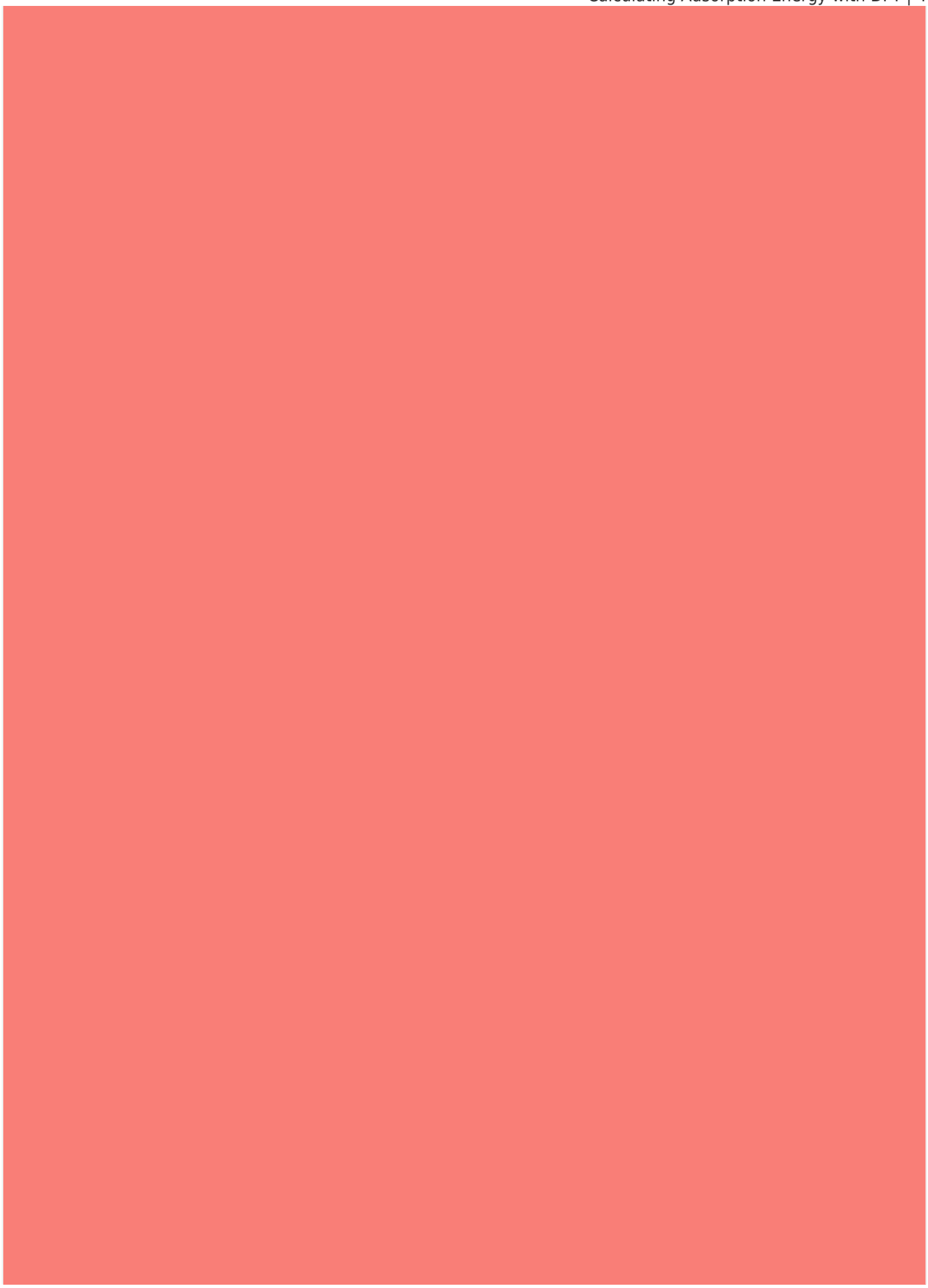

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