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|  |  |  הטכניון - מכון טכנולוגי לישראל TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY |
| הפקולטה להנדסה כימיתע"ש וולפסון |  |  |
| The Wolfson Department of Chemical Engineering |  |  |

**Wolfson Department of Chemical Engineering Seminar**

**Wednesday, February 23rd, 2022 at 13:30**

**Zoom:** <https://technion.zoom.us/j/97577956516>

**Is there (Regio) selectivity in polymer mechanochemical C-C bond scission?**

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**M.Sc. Seminar**

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# Abstract

Stable carbon-carbon bonds can be broken in a metathesis cracking process, however, this process is non-selective and very energy expensive. C-C bonds were also shown to be cleaved easily using mechanical stress in polymers (mechanochemistry); however, this is also not a selective process. This research aims at finding a way to manipulate the mechanical scission of a C-C bond and make it regioselective. More than 40 different structures were tested *in silico* using the Constrained Geometry simulates External Force (CoGEF) method. It was found that carbon substituents can reduce the required force for bond scission by up to 10%, while changing the bond angle leads to a reduction of up to 15%, and, finally, using a cyclooctane structure leads to significant force reductions of about 35%. Cis and trans isomers showed breaking force reduction only in cyclic structures, by up to 15%. The cyclooctane structure which offered the highest chance of presenting selective C-C bond scission was validated experimentally by introducing it in polyphthalaldehyde. Three different polyphthalaldehydes were prepared and their mechanochemical depolymerization kinetics compared, with the two controls supporting a selective C-C bond scission in the polymer with the cyclooctane. This work had emphasizes the challenges in accomplishing a regioselective C-C bond scission in polymers, but provides fundamental understanding on how different structural parameters can lead to such selectivity, especially if used in combination.