

SUPPLEMENTARY MATERIAL

Machine Learning Approach to Predict Physical Properties of Polypropylene Composites:

Application of MLR, DNN, and Random Forest to Industrial Data

Chonghyo Joo ^{1,2,†}, Hyundo Park ^{1,2,†}, Hyukwon Kwon ^{1,2}, Jongkoo Lim ³, Eunchul Shin ³, Hyungtae Cho ¹ and Junghwan Kim ^{1,*}

¹ *Green Materials and Processes R&D Group, Korea Institute of Industrial Technology, 55, Jongga-ro, Jung-gu, 44413 Ulsan, Korea*

² *Department of Chemical and Biomolecular Engineering, Yonsei University, 50, Yonsei-ro, Seodaemun-gu, 03722 Seoul, Korea*

³ *Research & Development Center, GS Caltex Corporation, 359, Expo-ro, Yuseon-gu, 34122 Daejeon, Korea*

[†] **Co-first authors: These authors contributed equally to this work.**

***Corresponding author**

Junghwan Kim

E-mail: kjh31@kitech.re.kr

Table S1. Pseudo code of categorization

Algorithm: Categorization		
<hr/>		
Input: \mathcal{M} : $n \times d$ recipe dataset, n : Number of recipes, d : Number of materials.		
Output: \mathcal{C} : Category set.		
<hr/>		
1:	Binning process	
2:	for each $u \in \mathcal{M}$ do	
3:	if $u > 0$ //	If u is bigger than zero, replace the value of u with “T.”
4:	replace u value with “T”	
5:	if $u = 0$ //	If u is zero, replace the value of u with “F.”
6:	replace u value with “F”	
7:	end	
8:	$\mathcal{M} \rightarrow \mathcal{M}'$ //	Recipe dataset replaced with “T” and “F” after binning process.
9:	Categorization process	
10:	for each $u \in \mathcal{M}'$ do	
11:	arrange u from $u(n, 1)$ to $u(n, d)$ //	Make code a consisting of “T” and “F.”
12:	give the arranged code a to data point $(n,)$ //	Give code a to each recipe.
13:	for each code $a \in \mathcal{M}'$ do	
14:	for each code $b \in \mathcal{M}' \setminus u$ do	
15:	if $a = b$ //	If a and b are same, add the recipes to the same category
16:	add (a, b) pair to the same category in the category set \mathcal{C}	
16:	Return \mathcal{C}	
