Supplementary Information

Molybdenum Incorporated Mesoporous Silica Catalyst for Production of Biofuels and Value-added Chemicals via Catalytic Fast Pyrolysis

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Table S1: Total acidity of catalysts evaluated from NH₃-TPD and Bronsted and Lewis acidity based on pyridine DRIFTS and ammonia chemisorption.

| Catalyst | Total Acidity (μmol g ⁻¹) | Bronsted Acidity (μmol g ⁻¹) | Lewis Acidity (µmol g ⁻¹) |
|----------|--|---|--|
| 0.25g-Mo | 55 | 2 | 53 |
| 1g-Mo | 77 | 1 | 76 |
| 2g-Mo | 98 | 2 | 96 |

Table S2: Elemental composition of catalyst from EDS analysis

| Catalyst | Oxygen (wt %) | Silicon (wt %) | Molybdenum (wt %) |
|----------|-----------------|-----------------|-------------------|
| 0.25g-Mo | 32.7 ± 6.8 | 61.1 ± 5.7 | 6.1 ± 1.9 |
| 1g-Mo | 30.8 ± 8.6 | 66.1 ± 8.6 | 3.1 ± 0.5 |
| 2g-Mo | 31.8 ± 11.8 | 63.0 ± 14.7 | 5.2 ± 8.0 |

Table S3: List of compounds identified by py-GCMS through fast pyrolysis of pine using 2g-Mo catalyst at biomass to catalyst ratio of 1:10

| m/z | Compound | Structure |
|-----|---------------------|-----------------|
| 16 | methane | CH ₄ |
| 18 | Water | н,0,н |
| 40 | Propyne | |
| 42 | Propene | |
| 44 | Acetaldehyde | \sim_0 |
| 44 | Carbon dioxide | 0=C=0 |
| 54 | Cyclobutene | |
| 56 | 2-propenal | 0 |
| 58 | Acetone | |
| 60 | Acetic acid | ОН |
| 66 | 1,3-cyclopentadiene | |

| 66 | 1-Buten-3-yne, 2-methyl- | |
|----|------------------------------------|---------------------------|
| 68 | Furan | |
| 70 | 2,3-dihydrofuran | |
| 70 | 3-buten-2-one | |
| 70 | 2-butenal | 0 |
| 72 | 2-butanone | |
| 74 | Propanoic acid | ОН |
| 78 | Benzene | \bigcirc |
| 78 | Cyclopenetene, 1- methyl- | |
| 80 | 1,3-cyclopentadiene, 1- methyl- | |
| 82 | Furan, 2-methyl- | |
| 84 | 3-buten-2-one, 3-methyl- | $\mathbf{M}^{\mathbf{O}}$ |
| 84 | 3-penten-2-one | |
| 86 | Butyrolactone | |

| 94 | Phenol | ОН |
|-----|--|----|
| 96 | Furan, 2,5-dimethyl- | |
| 96 | Furfural | |
| 96 | 2-cyclopentene-1,4- dione | |
| 96 | 2-cyclopenten-1-one, 2- methyl- | |
| 106 | p- xylene | |
| 108 | Phenol, 3-methyl- | НО |
| 116 | Indene | |
| 118 | Benzofuran | |
| 130 | 1H-Indene, 1-methyl- | |
| 134 | Benzene, 1-methyl-4-(1- methylethyl)- | |
| 134 | Benzene, 1-methyl-2-(1- methylethyl)- | |

| 170 | Naphthalene, 1,4,6,- trimethyl- | |
|-----|---|--|
| 234 | Phenanthrene, 1-methyl- 7-(1-methylethyl)- | |



Figure S1. Pore size distribution profiles of all three catalysts calculated by the BJH method.



Figure S2. Temperature programmed desorption profile of ammonia for the catalysts investigated for fast pyrolysis of biomass and its biopolymers cellulose and lignin. Profiles are offset for clarity



Figure S3. EDS mapping of 1g-Mo catalyst particles used to measure dispersion of active species within the catalysts.



Figure S4. Nitrogen adsorption and desorption isotherm of KIT-5 mesoporous silica support.