

**FIRST PRINCIPLE CALCULATIONS OF DEFECT STRUCTURES
IN ZINC OXIDE**

By

CHRISTIAN LOER T. LLEMIT

An undergraduate thesis submitted in partial fulfillment of
the requirements for the degree of

BACHELOR OF SCIENCE IN APPLIED PHYSICS

NATIONAL INSTITUTE OF PHYSICS
University of the Philippines - Diliman

MAY 2020

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To the Faculty of University of the Philippines Diliman National Institute of Physics:

The members of the Committee appointed to examine the thesis of CHRISTIAN LOER
T. LLEMIT find it satisfactory and recommend that it be accepted.

Roland V. Sarmago, Ph.D., Chair

Donald Trump, Ph.D.

Rodrigo Duterte, Ph.D.

ACKNOWLEDGMENT

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FIRST PRINCIPLE CALCULATIONS OF DEFECT STRUCTURES
IN ZINC OXIDE

Abstract

by Christian Loer T. Llemit, BS
University of the Philippines - Diliman
May 2020

: Roland V. Sarmago

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Dedication

This dissertation/thesis is dedicated to my mother and father who
provided both emotional and financial support

Chapter One

INTRODUCTION

1.1 Purpose and Motivation

Describe the importance of defects in ZnO

1.2 Objectives

Study the mechanisms of different defects in ZnO

1.3 Outline

This is an example of how to cite [\[1\]](#)

Chapter Two

Review of Related Literature

2.1 Semiconductors

2.1.1 Properties

2.1.2 Applications of Semiconductors

2.1.3 Defects in Semiconductors

2.2 Zinc Oxide

describe ZnO in broad perspective

2.2.1 Crystal Structure

Consider different phases

2.2.2 Crystallographic Directions and Planes

2.2.3 Brillouin Zone Symmetry

2.2.4 Photoluminescence Properties

2.2.5 Defects

Chapter Three

THEORETICAL FRAMEWORK

3.1 Electronic Structure

3.1.1 Electronic Bandstructure

3.1.1.1 Bloch Wavefunctions

insert the symmetry points in IBZ.

3.1.2 Density of States

explains fermi dirac distribution

3.1.3 Projected Density of States

3.2 Many-body Quantum Mechanics

insert text here

3.2.1 Time Independent Schrödinger Equation

3.2.2 Simplifying Assumptions

3.2.3 Use of Atomic Units

3.2.4 Hamiltonian Operator

3.2.5 Indistinguishability of electrons

3.3 Early First Principle Calculations

3.3.1 n-electron problem

3.3.2 Hartree Method

3.3.3 Hartree-Fock Method

3.4 Density Functional Theory

3.4.1 Electron Density

3.4.2 Hohenberg-Kohn (HK) Formalism

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3.4.3 Kohn Sham (KS) Formalism

3.4.3.1 KS Equation

3.4.3.2 Energy Terms

3.4.4 Self Consistent Field Calculation

3.5 Exchange-correlation Functional

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DFT Calculation of Solids

4.1 Basis Sets

4.1.1 Plane Wave

4.1.2 Gaussian Orbital

4.1.3 Slater type orbitals

4.2 Pseudopotential Approach

This is sample text

4.2.1 Freezing the core electrons

4.2.2 Pseudizing the valence electrons

4.2.3 Common Pseudopotentials

4.2.3.1 Norm-Conserving PP

4.2.3.2 Ultrasoft PP

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4.3 Choosing the appropriate Calculation Size

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4.3.2.1 Reciprocal Lattice

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4.3.3 k-point sampling

4.3.3.1 Monkhorst-Pack method

4.3.3.2 Gamma Point Sampling

Example of double quotes “word”. Lore

4.4 Bloch Representations

4.4.1 Electrons in solid

4.4.2 Bloch Theorem in periodic systems

4.4.3 Fourier Expansion of Bloch representations

4.4.3.1 Fourier Expansions

4.4.3.2 Fast Fourier Transformation (FFT)

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4.5 Plane Wave (PW) Expansion

4.5.1 Basis Set

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4.5.2.3 Effective Potential

4.6 Electronic Structure

4.6.1 Band Structure of free electrons

4.6.2 Band Structure of electrons in solids

4.6.3 Electronic Density of States

4.7 Practical Aspects

Chapter Five

Software Implementation

5.1 QUANTUM ESPRESSO

5.1.1 MKL Libraries

5.1.2 PWSCF routines

cbands, cegterg, cdiaghg

5.2 Intel Compilers

5.3 Executables

5.4 Computational Details

5.4.1 Convergence Testing

5.4.2 Hubbard correction parameters

5.4.3 Supercell creation

5.4.4 Slab Model

5.4.5 Structural relaxation

5.4.6 scf calculation

5.4.7 bandstructure calculation

5.4.8 dos calculation

DOST COARE

Chapter Six

MATHEMATICS NOTATION

6.1 Some Math Stuff

LaTeX has a special way to embed mathematical symbols and notations. Here are some of them. Also observe how a bullet list is made.

- greater than \geq
- less than \leq
- percent sign %
- multiply $N \times N$
- inline equation $M = N(N - 1)/2$

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6.2 Math equation

Example of a mathematical formula:

$$ADD = \sum_{i=1}^M | < D(n+1, i) > - < D(n, i) > | \quad (6.1)$$

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6.3 Chapter section

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6.4 Chapter section

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Chapter Seven

FIGURES AND TABLES

7.1 Examples of a figure

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Example of a figure. Example of reference to a figure in the text (Fig. 7.1). Phasellus dolor neque, vehicula vestibulum semper at, facilisis eget libero. Mauris interdum magna molestie, auctor felis a, condimentum odio. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Suspendisse maximus lacinia dignissim. Maecenas pharetra accumsan metus, sagittis dictum purus sollicitudin eget. Curabitur ut porttitor arcu, ut porttitor ipsum. Vestibulum porttitor finibus sapien, ac pharetra odio bibendum nec. Nullam tincidunt dignissim risus imperdiet dictum.

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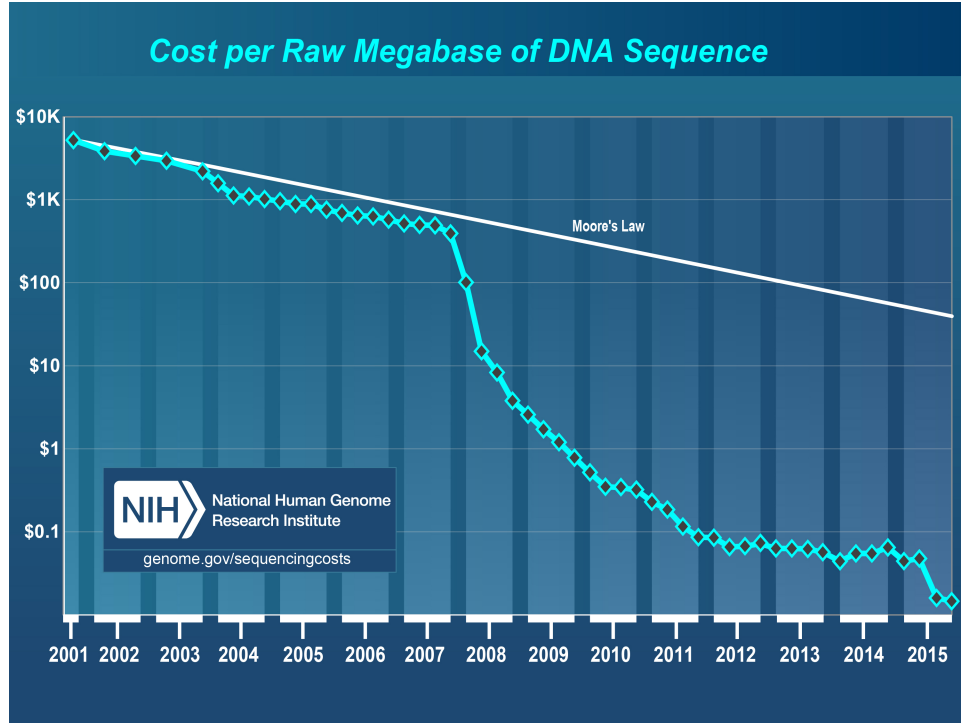


Figure 7.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [2]

7.2 Example of a table

Example of a table and here is the reference to Table 7.1. Tables in, my opinion, are the hardest thing to make.

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ORGANISM	ACCESSION NO.	GENOME SIZE (bp)	No. CDS
<i>Mesorhizobium loti</i>	NC_002678	7036071	6743
<i>Sinorhizobium meliloti</i>	NC_003047	3654135	3359
<i>Bradyrhizobium japonicum</i>	NC_004463	9105828	8317
<i>Rhodopseudomonas palustris</i>	NC_005296	5459213	4813
<i>Bartonella quintana</i>	NC_005955	1581384	1142
<i>Bartonella henselae</i>	NC_005956	1931047	1488
<i>Rickettsia typhi</i>	NC_006142	1111496	837
<i>Beijerinckia indica</i>	NC_010581	4170153	3569

Table 7.1 Whole-genome sequences used in this study

sapien, ac pharetra odio bibendum nec. Nullam tincidunt dignissim risus imperdiet dictum.

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7.3 Chapter section

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maximus lacinia dignissim. Maecenas pharetra accumsan metus, sagittis dictum purus sollicitudin eget. Curabitur ut porttitor arcu, ut porttitor ipsum. Vestibulum porttitor finibus sapien, ac pharetra odio bibendum nec. Nullam tincidunt dignissim risus imperdiet dictum.

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REFERENCES

1. Prades, J. D., Cirera, A. & Morante, J. R. Ab initio calculations of NO₂ and SO₂ chemisorption onto non-polar ZnO surfaces. *Sensors and Actuators, B: Chemical* **142**, 179–184 (1 Oct. 2009).
2. Wetterstrand, K. A. *DNA Sequencing Costs: Data from the NHGRI Genome Sequencing Program (GSP)* www.genome.gov/sequencingcosts.

APPENDIX

Appendix A

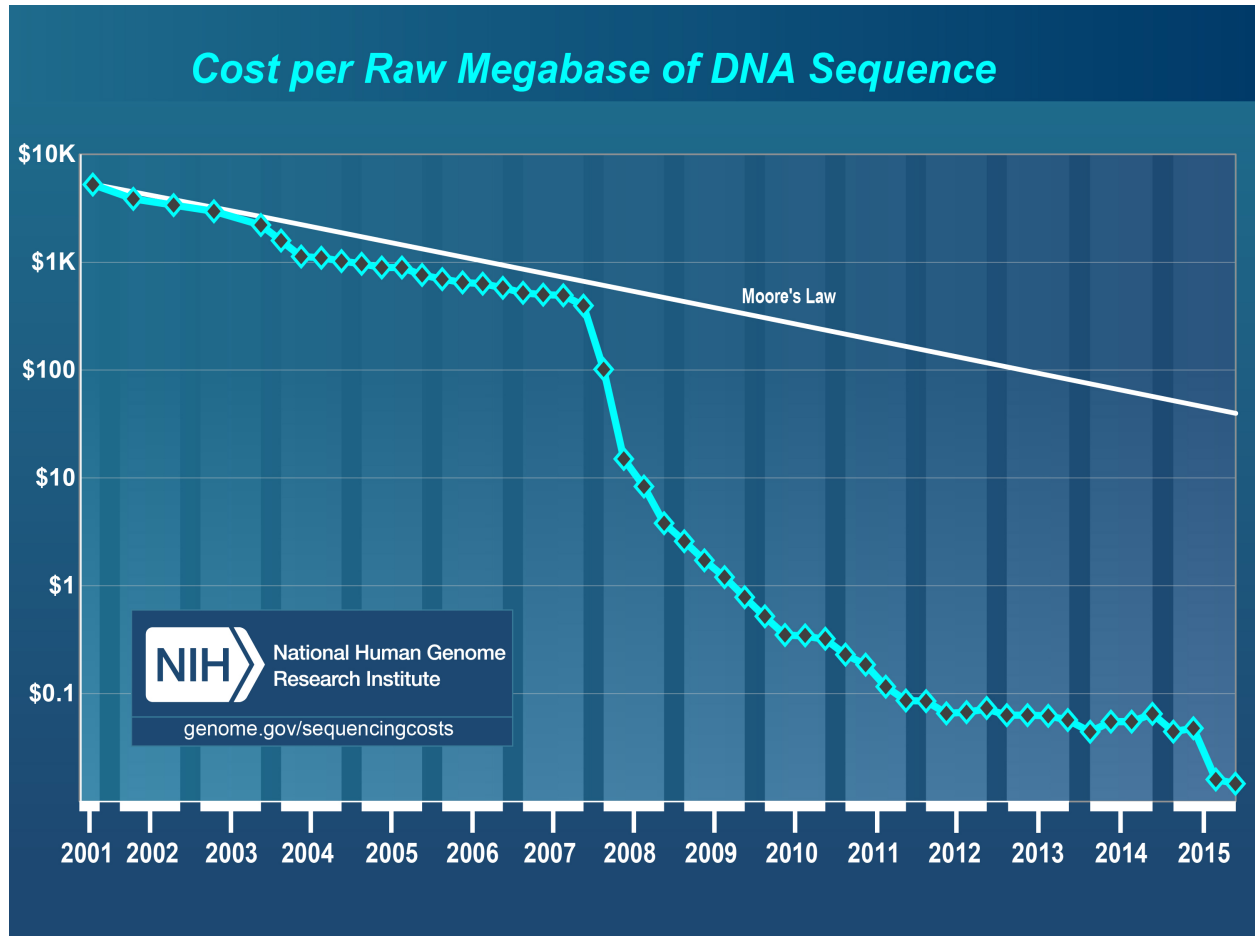


Figure A.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [2]

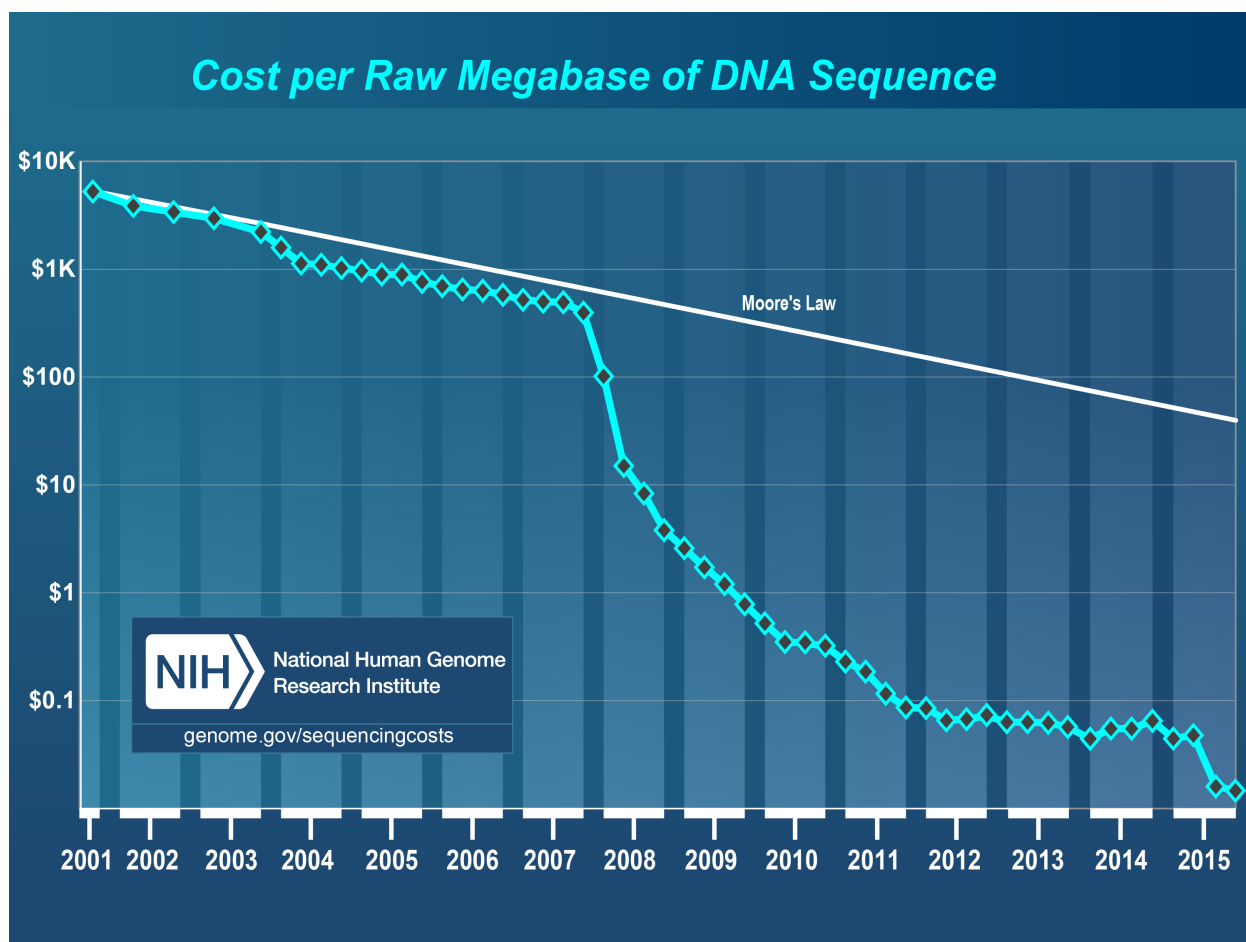


Figure A.2 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [2]

Appendix B

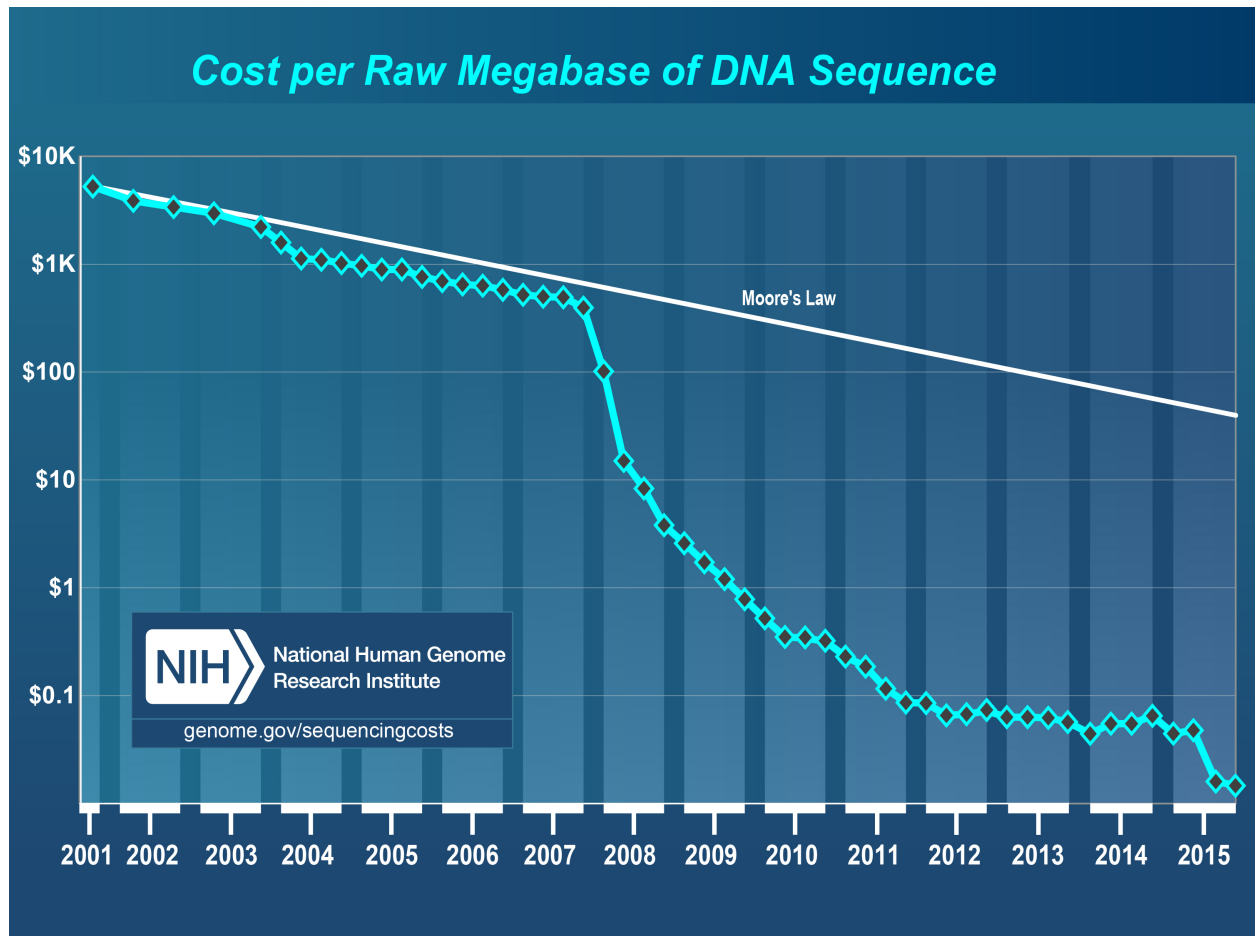


Figure B.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [2]

Appendix C

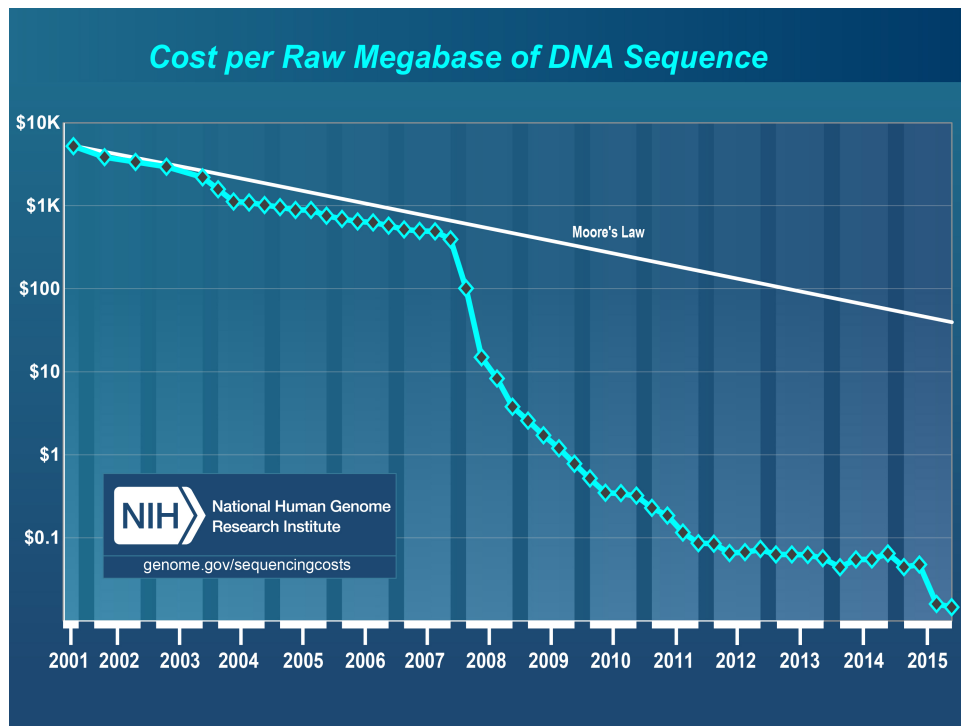


Figure C.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [2]

Appendix D

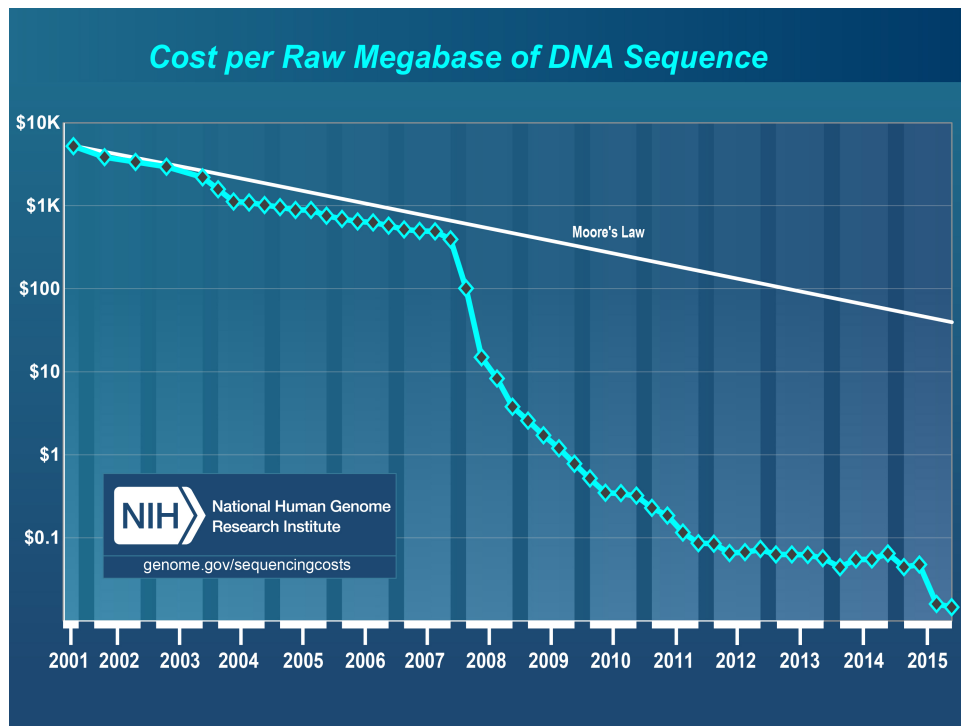


Figure D.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [2]

Appendix E

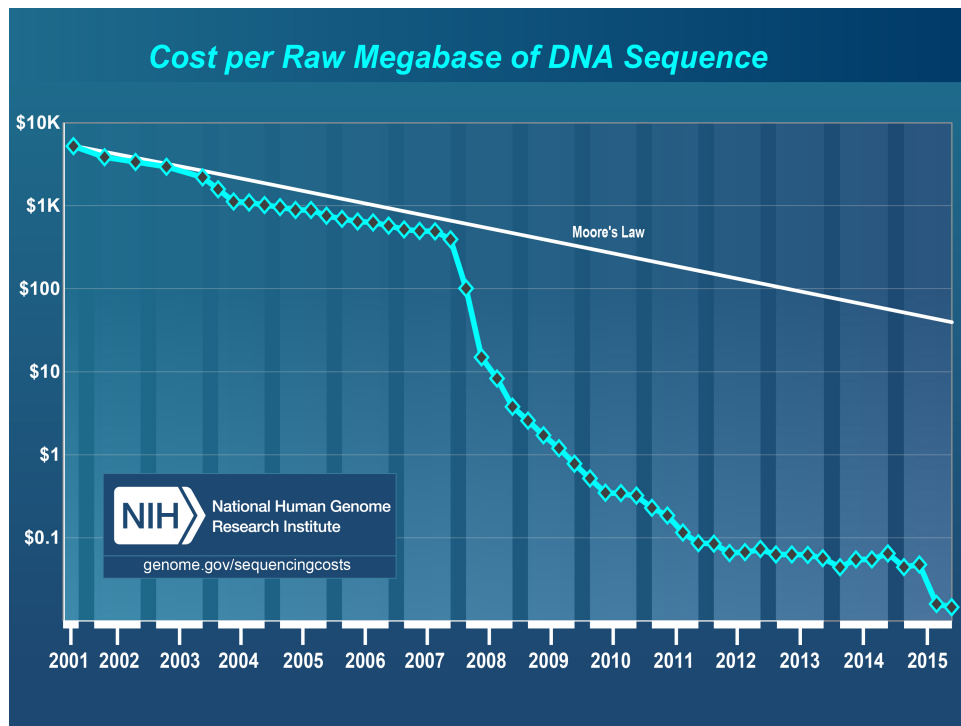


Figure E.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [2]